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DOCUMENTATION OF SED--A SEDIMENT/WATER COLUMN CONTAMINANT MODEL

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ERRATA

The authors wish to add this information to NOAA Technical Memorandum ERL GLERL-41, ***Documentation*** of *SED--A Sediment/Water Column Contaminant Model*, August 1982, by Gregory A. Lang and Steven C. Chapra.

The FORTRAN program listed in Appendix B was written for a CDC Cyber 750 FORTRAN Extended Version 4.8 compiler. Successful application of this code to other compilers is not guaranteed.

In addition, the authors wish to reference the two software packages used in the program. The first package is the IMSL Library, Edition 9. It is a product of International Mathematical and Statistical Libraries, Incorporated, NBC Building, 7500 Bellaire Blvd., Houston, Texas. The subroutine ZSYSTM, called on page 41, Appendix B, was used from this package to simultaneously solve a set of non-linear equations. ZSYSTM has subsequently been replaced in the IMSL Library by the subroutine ZSPOW. The second software package is the DISSPLA version 8.2 software system. It is a product of the Integrated Software Systems Corporation (ISSCO), 4186 Sorrento Valley Blvd., San Diego, California. The subroutines called on pages 46 and 47, Appendix B, (excluding the subroutine RMAX) are all part of DISSPLA and were used to generate the plots in figures 4 and 5.

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DOCUMENTATION OF SED--

A SEDIMENT/WATER COLUMN CONTAMINANT MODEL*

Gregory A. Lang and Steven C. Chapra

Presented is documentation of a mathematical model developed to simulate the contaminant level in the sediments and overlying water column of a well-mixed lake. The contaminant is segmented into three fractions, organic, inorganic, and dissolved, each with different physical and kinetic properties. The principal application of the model would be prediction of the year-to-year and steady-state response of the water column and sediments to changes in the loading rate of contaminant and/or particulate matter. A simulation of ^{239}Pu in Lake Michigan is presented as an example of the model's use.

1. INTRODUCTION

Presented here is a brief description of a sediment/water column contaminant model called SED. It was developed by Dr. Steven Chapra, now a Professor at Texas A & M University, while he was at NOAA, Great Lakes Environmental Research Laboratory. Much of his work dealing with this model appears in "Long-term models of interactions between solids and contaminants in lakes" (Chapra,1982), and ***Engineering Approaches for Luke** Management--* ***Vol. 2: Mechanistic Modeling*** (Chapra and Reckhow, 1982).

SED is a mathematical model designed to simulate the concentration of a contaminant in the sediments and overlying water column of a lake. It operates on an annual time scale, ignoring within-year variations. Its principal application would be to predict the year-to-year and steady-state responses of the water column and sediments to changes in the amount of contaminant and/or particulate matter entering the lake.

2. MODEL DEVELOPMENT

The contaminant being considered is divided into three components--that associated with organic particulate matter, that associated with inorganic particulate matter, and that dissolved in the water. Adsorption/desorption plays an important role in such a kinetic segmentation scheme because only the portion of a contaminant that associates with particulate matter is subject to settling and resuspension and only the dissolved component is subject to diffusion and vaporization.

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*GLERL Contribution No. 325.

The water column is idealized as a completely mixed volume resulting in a lake-wide average contaminant concentration. The sediments are horizontally subdivided into well-mixed "slices" varying in thickness from a half of a centimeter near the sediment/water interface to several meters in the deep sediment. This spatial segmentation scheme (figure 1) yields a lake-wide mean annual estimate of the level of contaminant in the water column and provides the vertical profile of contaminant in the sediments.

SED comprises two main parts--a solids budget and a contaminant budget. The solids budget uses information such as the loading rate of particulate matter, density and porosity of the sediments, and various settling rates to calculate the steady-state concentrations of organic and inorganic particulate matter in the water column and sediments, as well as the burial velocity (or sedimentation rate). The contaminant budget uses information such as the physical characteristics of the lake, the loading rate and kinetic properties of the contaminant, and the results of the solids budget to predict the concentration of the three forms of contaminant in the water column and sediments. See flow chart in figure 2.

2.1 Contaminant Budget

The contaminant budget consists of a set of coupled differential equations that result when mass balances are written for each of the three contaminant components within their respective "pools." A pool is simply a place of residence, so to speak, for each of the three components. Each

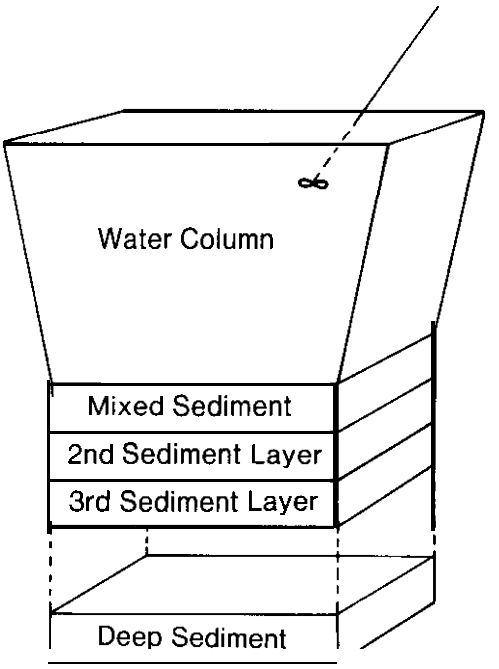

FIGURE 1.--*Spatial* ***segmentation scheme used*** *in* ***SED.***

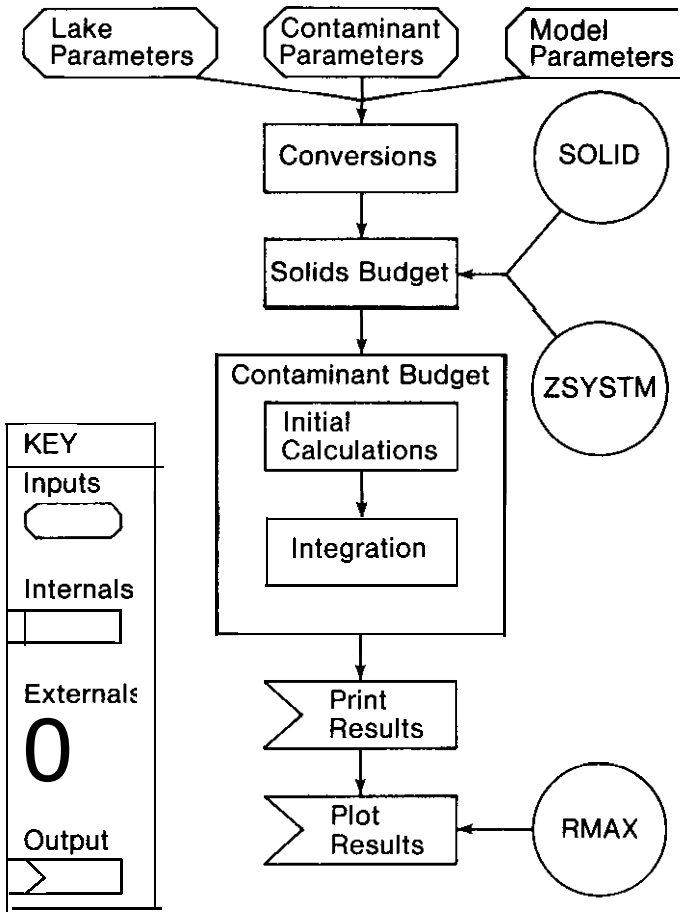

FIGURE 2.--*Flow chart representing the pathways of SED.*

well-mixed volume comprises three such pools--the organic solids volume (organic pool), the inorganic solids volume (inorganic pool), and the liquid volume (liquid pool). Contaminant levels within the three pools in each control volume depend on system inputs, system losses, and interactions between pools. Inputs are in the form of contaminant loading; losses include flushing, settling, vaporization, and decay; and interactions between pools consist of adsorption and desorption, resuspension, settling, and diffusion. See figure 3.

2.1.1 Water Column Balance

The term "water column" is somewhat imprecise--it refers to the entire lake volume, which includes all three pools, and not just to the liquid pool, as the term might suggest. But, since the porosity of the water column is assumed to be equal to one, the ***volume*** of the liquid pool is, in fact, essentially equal to the volume of the entire water column. This distinction is important in the sediments where the porosity is less than one. Presented below are the differential equations for the three pools in the water column and for the entire water column.

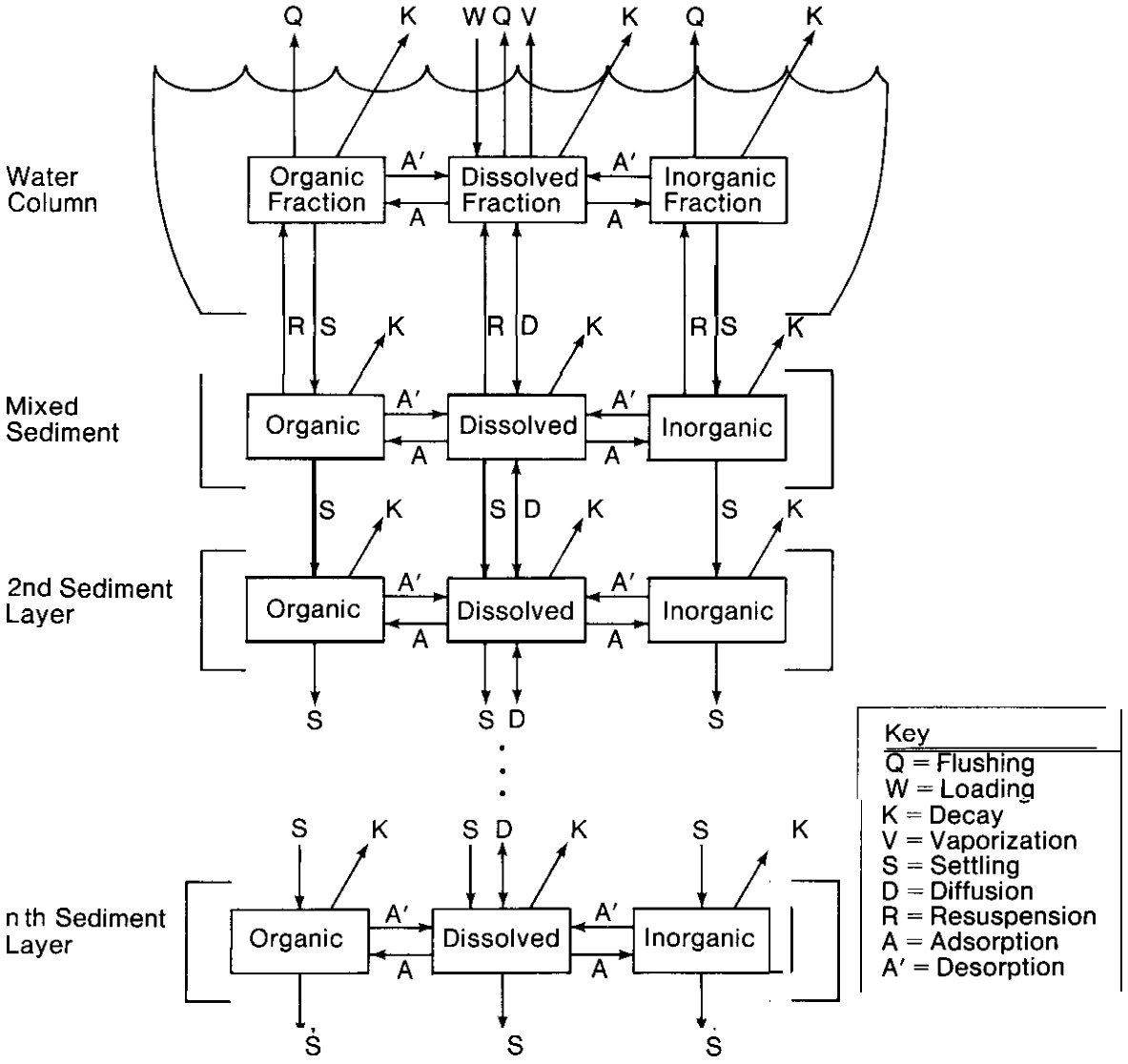

FIGURE 3.--*Overview of contaminant* ***budget.*** *Arrows* ***represent pathways of contaminant into and out of the system, between control volumes, and*** *between* ***pools.***

2.1.1.1 Organic Pool. A mass balance for the contaminant associated with the organic solids in the water column can be written as

$$m_{o,w}\frac{d\nu_{o,w}}{dt} = k_{ad,o,w}\, m_{o,w}\, c_{1,w} - k_{de,o,w}\, m_{o,w}\, \nu_{o,w} - \frac{Q}{V_{t,w}}\, m_{o,w}\, \nu_{o,w}$$

(absorption) (desorption) (flushing)

$$\frac{v_{o,w} A_w}{V_{t,w} m_{o,w}}\, \nu_{o,w} + \frac{v_r A_m}{V_t m_m}\, m_{o,m}\, \nu_{o,m} - k_{o,w}\, m_{o,w}\, \nu_{o,w}, \qquad (1)$$

(settling) (resuspension) (decay)

where $m_{o,w}$ = mass of organic suspended solids, grams dry weight*,

$\nu_{o,w}$ = curies** of contaminant associated with the organic solids per mass of organic solid, curies per gram,

$k_{ad,o,w}$ = adsorption rate of contaminant from liquid pool to organic pool, cubic meters per gram per year,

$k_{de,o,w}$ = desorption rate of contaminant from organic pool to liquid pool, per year,

$c_{1,w}$ = curies of contaminant dissolved in liquid pool per volume of liquid pool, curies per cubic meter,

Q = advective water flow leaving lake, cubic meters per year,

$V_{t,w}$ = volume of water column, cubic meters,

$v_{o,w}$ = settling rate of organic solids, meters per year,

A_w = average surface area of the water column, square meters,

v_r = resuspension rate, meters per year,

A_m = surface area at sediment/water interface, square meters,

---

*For simplicity, the term "dry weight" will be dropped, and henceforth the term gram will stand for "grams dry weight" unless otherwise noted.

**Keep in mind that not all contaminants are measured in curies (e.g., PCB's are measured in mass units, such as μg).

$V_{t,m}$ = volume of first sediment layer (mixed sediment), cubic meters,

$m_{o,m}$ = mass of organic solids in mixed sediment, grams,

$\nu_{o,m}$ = curies of contaminant associated with the organic solids in the mixed sediment per mass of organic solid, curies per gram,

$k_{o,w}$ = decay rate of contaminant in the organic pool, per year,

t = time, years, and

w = subscript denoting water column.

2.1.1.2 Inorganic Pool. A mass balance for the contaminant associated with the inorganic solids in the water column can be written as

$$m_{i,w} \frac{d\nu_{i,w}}{dt} = k_{ad,i,w} \quad m_{i,w} \quad c_{1,w} \quad k_{de,i,w} \quad m_{i,w} \quad \nu_{i,w} - \frac{Q}{V_{t,w}} m_{i,w} \nu_{i,w}$$

(adsorption) (desorption) (flushing)

$$\frac{v_{i,w} A_w}{V_{t,w}} m_{i,w} \nu_{i,w} + \frac{v_r A_m}{V_{t,m}} m_{i,m} \quad \nu_{i,m} \quad k_{i,w} \quad m_{i,w} \quad \nu_{i,w}, \qquad (2)$$

(settling) (resuspension) (decay)

where the terms are identical to the terms for the organic pool, except that the subscript "o" has been replaced by the subscript "i," denoting inorganic.

2.1.1.3 Liquid Pool. A mass balance for the contaminant dissolved in the liquid pool can be written as

$$V_{1,w} \frac{dc_{1,w}}{dt} = W_c(t) - Q c_{1,w} - v_v A_s c_{1,w} + k_{de,o,w} m_{o,w} \nu_{o,w}$$

(loading) (flushing) (vaporization) (desorption)

$$- k_{ad,o,w} m_{o,w} c_{1,w} + k_{de,i,w} m_{i,w} \nu_{i,w} - k_{ad,i,w} m_{i,w} c_{1,w}$$

(adsorption) (desorption) (adsoprtion)

$$+ \frac{\phi E_s A_m}{(z_b+z_m)/2} \left(c_{pw,m} - c_{1,w}\right) + v_r \phi A_m c_{pw,m} - k_{d,w} V_{1,w} c_{1,w}, \qquad (3)$$

(diffusion) (resuspension) (decay)

where $V_{l,w}$ = volume of the liquid pool, cubic meters,

$W_c(t)$ = loading rate of contaminant dissolved in the liquid pool, curies per year,

v_v = vaporization rate, meters per year,

A_s = surface area at air/water interface, square meters,

ϕ = porosity of sediments, dimensionless,

E_s = diffusion coefficient, square meters per year,

z_b = thickness of the laminar boundary layer above the sediment/water interface, meters,

z_m = thickness of mixed sediment layer, meters,

$c_{pw,m}$ = curies of dissolved contaminant per volume of liquid pool in mixed sediment, curies per cubic meter, and

$k_{d,w}$ = decay rate of contaminant dissolved in liquid pool, per year.

Note that

$$E_s = E_m \phi^2,$$

where E_m = molecular diffusion, square meters per year.

2.1.1.4 Total Contaminant in the Water Column. It is often more desirable to work in terms of the total contaminant (i.e., the sum of the three components), thus reducing the number of equations per control volume to one and greatly simplifying the calculations. Since sorption reactions typically proceed much faster than input-output processes, a local equilibrium can be assumed and equations (1), (2), and (3) can be combined to yield

$$V_{t,w} \frac{dc_{t,w}}{dt} = W_c(t) - \frac{Q}{V_{t,w}} m_{o,w} \nu_{o,w} - \frac{Q}{V_{t,w}} m_{i,w} \nu_{i,w} - Q\, c_{l,w}$$

$$\frac{v_{o,w} A_s}{V_{t,w}} m_{o,w} \nu_{o,w} - \frac{v_{i,w} A_s}{V_{t,w}} m_{i,w} \nu_{i,w} - v_v A_s c_{l,w}$$

$$+ \frac{\phi E_s A_m}{z'_b} \left(c_{pw,m} - c_{l,w}\right) + \frac{v_r A_m}{V_{t,m}} m_{o,m} \nu_{o,m} + \frac{v_r A_m}{V_{t,m}} m_{i,m} \nu_{i,m}$$

$$+ v_r \phi A_m c_{pw,m} - k_{o,w} m_{o,w} \nu_{o,w} - k_{i,w} m_{i,w} \nu_{i,w} - k_{d,w} V_{l,w} c_{l,w}, \quad (4)$$

where $c_{t,w}$ = curies of total contaminant in water column per total volume of water column, curies per cubic meter, and

z_b' = thickness defining the gradient between the mixed sediment and the overlying Water $(=(z_b + z_m)/2)$,

Some new terms must be introduced to relate the individual terms $\nu_{o,w}$, $\nu_{i,w}$, and $c_{l,w}$ to the total concentration, $c_{t,w}$. Remember that, since the porosity of the water column is essentially equal to one, the volume of the liquid pool equals the volume of the water column, or

$$V_{l,w} = V_{t,w}.$$

And it follows that the concentration of dissolved contaminant with respect to the liquid pool, $c_{l,w}$, is essentially equal to the concentration of dissolved contaminant with respect to the total water column, or

$$c_{l,w} = c_{d,w},$$

where $c_{d,w}$ = curies of contaminant dissolved in liquid pool per total volume of water column, curies per cubic meter.

Defining the terms

$$c_{o,w} = \frac{m_{o,w} \nu_{o,w}}{V_{t,w}} \quad (5)$$

and

$$c_{i,w} = \frac{m_{i,w} \nu_{i,w}}{V_{t,w}} \quad (6)$$

where $c_{o,w}$ = curies of contaminant associated with organic solids per total water column volume, curies per cubic meter, and

$c_{i,w}$ = curies of contaminant associated with inorganic solids per total water column volume, curies per cubic meter,

yields an expression for the total contaminant in the water column in terms of its three components,

$$c_{t,w} = c_{d,w} + c_{o,w} + c_{i,w} \tag{7}$$

or

$$c_{t,w} = c_{d,w} + \frac{m_{o,w}\ \nu_{o,w}}{V_{t,w}} + \frac{m_{i,w}\ \nu_{i,w}}{V_{t,w}}. \tag{8}$$

In a temporal sense, many sorption reactions are rapid and are assumed to reach equilibrium much faster than the yearly time scale of the model. This equilibrium is a dynamic state representing a balance between adsorption and desorption, as in

$$k_{ad,o,w}\ m_{o,w}\ c_{d,w} = k_{de,o,w}\ m_{o,w}\ \nu_{o,w}$$

and

$$k_{ad,i,w}\ m_{i,w}\ c_{d,w} = k_{de,i,w}\ m_{i,w}\ \nu_{i,w}.$$

With the above assumption, the following partition coefficients can be defined:

$$K_{d,o,w} = \frac{k_{ad,o,w}}{k_{de,o,w}} = \frac{\nu_{o,w}}{c_{d,w}} \tag{9}$$

and

$$K_{d,i,w} = \frac{k_{ad,i,w}}{k_{de,i,w}} = \frac{\nu_{i,w}}{c_{d,w}}, \tag{10}$$

where $K_{d,o,w}$ = organic partition (or distribution) coefficient in the water column, cubic meters per gram, and

$K_{d,i,w}$ = inorganic partition (or distribution) coefficient in the water column, cubic meters per gram.

Equations (8), (9), and (10) can be combined and rearranged to yield

$$c_{d,w} = F_{d,w}\ c_{t,w}, \tag{11}$$

where $F_{d,w} = \dfrac{1}{1 + \dfrac{m_{o,w} K_{d,o,w}}{V_{t,w}} + \dfrac{m_{i,w} K_{d,i,w}}{V_{t,w}}}$,

and

$$c_{o,w} = F_{o,w} \; c_{t,w}, \tag{12}$$

where $F_{o,w} = \dfrac{\dfrac{m_{o,w} K_{d,o,w}}{V_{t,w}}}{1 + \dfrac{m_{o,w} K_{d,o,w}}{V_{t,w}} + \dfrac{m_{i,w} K_{d,i,w}}{V_{t,w}}}$

and

$$c_{i,w} = F_{i,w} \; c_{t,w}, \tag{13}$$

where $F_{i,w} = \dfrac{\dfrac{m_{i,w} K_{d,i,w}}{V_{t,w}}}{1 + \dfrac{m_{o,w} K_{d,o,w}}{V_{t,w}} + \dfrac{m_{i,w} K_{d,i,w}}{V_{t,w}}}$

Thus,

$$c_{1,w} = c_{d,w} = F_{d,w} \; c_{t,w}, \tag{14}$$

$$\nu_{o,w} = \frac{V_{t,w}}{m_{o,w}} F_{o,w} \; c_{t,w}, \tag{15}$$

and

$$\nu_{i,w} = \frac{V_{t,w}}{m_{i,w}} F_{i,w} \; c_{t,w}. \tag{16}$$

Note that

$$F_{d,w} + F_{o,w} + F_{i,w} = 1.$$

Finally, by substituting equations (14), (15), and (16) into equation (4), the total contaminant balance in the water column can be reexpressed as

$$V_{t,w} \frac{dc_{t,w}}{dt} = W_c(t) - Q c_{t,w} - v_s A_s F_{d,w} c_{t,w} - v_{o,w} A_w F_{o,w} c_{t,w}$$

$$- v_{i,w} A_w F_{i,w} c_{t,w} + \frac{\phi E_s A_m}{z_b'} \left(F_{pw,m} c_{t,m}^{*} - F_{d,w} c_{t,w}\right)$$

$$+ v_r A_m c_{t,m}^{**} - k_{d,w} V_{t,w} F_{d,w} - k_{o,w} V_{t,w} F_{o,w} c_{t,w}$$

$$- k_{i,w} V_{t,w} F_{i,w} c_{t,w}. \qquad (17)$$

2.1.2 Mixed Sediment Balance

The mixed sediment is the first segment below the water column and is usually between 1 and 2 cm in depth. It is so called because of the intense mixing, or bioturbation, caused by the benthic organisms that reside there. The mixed sediment also comprises three pools--the liquid pool (also called the pore water), the organic pool, and the inorganic pool. Presented below are the differential equations for the three pools in the mixed sediment.

2.1.2.1 Organic Pool. A mass balance for the contaminant associated with the organic solids in the mixed sediment can be written as

---

*It will be shown in the following section that $c_{pw,m} = F_{pw,m} c_{t,m}$.

**It will also be shown that the sum of the three resuspension terms equals $v_r A_m c_{t,m}$.

$$m_{o,m} \frac{d\nu_{o,m}}{dt} = k_{ad,o,m}\, m_{o,m}\, c_{pw,m} - k_{de,o,m}\, m_{o,m}\, \nu_{o,m} + v_{q,w}\, A_w\, F_{q,w}\, c_{t,w}$$

(adsorption) (desorption) (settling)

$$- \frac{v_b\, A_m}{V_{t,m}}\, m_{o,m}\, \nu_{o,m} - \frac{v_r\, A_m}{V_{t,m}}\, m_{o,m}\, \nu_{o,m} - k_{o,m}\, m_{o,m}\, \nu_{o,m}, \qquad (18)$$

(burial) (resuspension) (decay)

where $c_{pw,m}$ = curies of contaminant dissolved in pore water per volume of pore water, curies per cubic meter, and

v_b = burial velocity, meters per year.

The remaining terms are identical to the terms used for the organic pool in the water column, except that the subscript "w" has been replaced by the subscript "m," denoting mixed sediment.

2.1.2.2 Inorganic Pool. A mass balance for the contaminant associated with the inorganic solids in the mixed sediment can be written as

$$m_{i,m} \frac{d\nu_{i,m}}{dt} = k_{ad,i,m}\, m_{i,m}\, c_{pw} - k_{de,i,m}\, m_{i,m}\, \nu_{i,m} + v_{i,w}\, A_w\, F_{i,w}\, c_{t,w}$$

(adsorption) (desorption) (settling)

$$- \frac{v_b\, A_m}{V_{t,m}}\, m_{i,m}\, \nu_{i,m} - \frac{v_r\, A_m}{V_{t,m}}\, m_{i,m}\, \nu_{i,m} - k_{i,m}\, m_{i,m}\, \nu_{i,m}, \qquad (19)$$

(burial) (resuspension) (decay)

where the terms are identical to the terms used for the organic pool in the mixed sediment, except that the subscript "o" has been replaced by the subscript "i," denoting inorganic.

2.1.2.3 Liquid Pool. A mass balance for the contaminant dissolved in the pore water in the mixed sediment can be written as

$$V_{pw,m} \frac{dc_{pw,m}}{dt} = k_{de,o,m}\, m_{o,m}\, v_{o,m} - k_{ad,o\,m,}\, m_{o,m}\, c_{pw,m} + k_{de,i\,m,}\, m_{i\,m}\, v_{i,m}$$

(desorption) (adsorption) (desorption)

$$- k_{ad,i,m}\, m_{i,m}\, c_{pw,m} + \frac{\phi\, E_s\, A_m}{z_b'} \left(F_{d,w}\, c_{t,w} - c_{pw,m}\right)$$

(adsorption) (diffusion)

$$+ \frac{\phi\, E_s\, A_m}{z_{m,2}} \left(c_{pw,2} - c_{pw,m}\right) - v_b\, \phi\, A_m\, c_{pw,m} - v_r\, \phi\, A_m\, c_{pw,m}$$

(diffusion) (burial) (resuspension)

$$- k_{d,m}\, V_{pw,m}\, c_{pw,m}, \qquad (20)$$

(decay)

where $V_{pw,m}$ = volume of the pore water, cubic meters,

$c_{pw,2}$ = concentration of contaminant dissolved in the pore water in the second sediment layer, curies per cubic meter, and

$z_{m,2}$ = mixing zone between mixed sediment and second sediment layer (= $(z_m + z_2)/2$), meters.

The remaining terms are identical to the terms used for the liquid pool in the water column, except that the subscript "w" has been replaced by the subscript "m," denoting mixed sediment.

2.1.2.4 Total Contaminant in the Mixed Sediment. Again it is desirable to work in terms of the total contaminant; therefore, adding equations (18), (19), and (20) yields

$$V_{t,m} \frac{dc_{t,m}}{dt} = v_{o,w}\, A_w\, F_{o,w}\, c_{t,w} + v_{i,w}\, A_w\, F_{i,w}\, c_{t,w}$$

$$+ \frac{\phi\, E_s\, A_m}{z_b'} \left(F_{d,w}\, c_{t,w} - c_{pw,m}\right) + \frac{\phi\, E_s\, A_m}{z_{m,2}} \left(c_{pw,2} - c_{pw,m}\right)$$

$$- \frac{v_b A_m}{V_{t,m}} m_{o,m} \nu_{o,m} - \frac{v_b A_m}{V_{t,m}} m_{i,m} \nu_{i,m} - v_b \phi A_m c_{pw,m}$$

$$- \frac{v_r A_m}{V_{t,m}} m_{o,m} \nu_{o,m} - \frac{v_r A_m}{V_{t,m}} m_{i,m} \nu_{i,m} - v_r \phi A_m c_{pw,m}$$

$$- k_{d,m} V_{pw,m} c_{p,m} k_{o,m} m_{o,m} \nu_{o,m} - k_{i,m} m_{i,m} \nu_{i,m}, \tag{21}$$

where $c_{t,m}$ = curies of total contaminant in mixed sediment per total volume of mixed sediment, curies per cubic meter.

It is again necessary to relate the individual terms $\nu_{o,m}$, $\nu_{i,m}$, and $c_{pw,m}$ to the total concentration, $c_{t,m}$. The volume of the pore water can be related to the total volume of the mixed sediment by the porosity, as in

$$V_{pw,m} = \phi V_{t,m}.$$

The concentration of contaminant dissolved in the pore water can also be related by porosity to the concentration of contaminant dissolved in the total mixed sediment volume, as in

$$c_{d,m} = \phi c_{pw,m}, \tag{22}$$

where $c_{d,m}$ = curies of contaminant dissolved in the pore water per total volume of mixed sediment, curies per cubic meter.

Defining the terms

$$c_{o,m} = \frac{m_{o,m} \nu_{o,m}}{V_{t,m}} \tag{23}$$

and

$$c_{i,m} = \frac{m_{i,m} \nu_{i,m}}{V_{t,m}}, \tag{24}$$

where $c_{o,m}$ = curies of contaminant associated with organic solids per total volume of mixed sediment, curies per cubic meter, and

$c_{i,m}$ = curies of contaminant associated with inorganic solids per total volume of mixed sediment, curies per cubic meter,

yields an expression for the total contaminant in the mixed sediment in terms of its three components as follows:

$$c_{t,m} = c_{d,m} + c_{o,m} + c_{i,m} \tag{25}$$

or

$$c_{t,m} = \phi c_{pw,m} + \frac{m_{o,m}\ \nu_{o,m}}{V_{t,m}} + \frac{m_{i,m}\ \nu_{i,m}}{V_{t,m}}. \tag{26}$$

Equation (26) can be further simplified by the use of the following equations:

$$\frac{m_{o,m}}{V_{t,m}} = \rho_o\ \phi_o \tag{27}$$

and

$$\frac{m_{i,m}}{V_{t,m}} = \rho_i\ \phi_i, \tag{28}$$

where ρ_o = mass density of the organic solids in the mixed sediment, grams per cubic meter,

ϕ_o = volume of the organic solids per total mixed sediment volume, dimensionless,

ρ_i = mass density of the inorganic solids in the mixed sediment, grams per cubic meter, and

ϕ_i = volume of the inorganic solids per total mixed sediment volume, dimensionless.

Note that

$$\phi + \phi_o + \phi_i = 1.$$

Thus,

$$c_{t,m} = \phi c_{pw,m} + \rho_o \phi_o \nu_{o,m} + \rho_i \phi_i \nu_{i,m}. \tag{29}$$

Again, partition coefficients are defined as

$$K_{d,o,m} = \frac{k_{ad,o,m}}{k_{de,o,m}} = \frac{\nu_{o,m}}{c_{pw,m}} \tag{30}$$

$$K_{d,i,m} = \frac{k_{ad,i,m}}{k_{de,i,m}} = \frac{\nu_{i,m}}{c_{pw,m}}, \tag{31}$$

where $K_{d,o,m}$ = organic partition coefficient, cubic meters per gram, and

$K_{d,i,m}$ = inorganic partition coefficient, cubic meters per gram.

Equations (29), (30), and (31) can be combined and rearranged to yield

$$c_{pw,m} = F_{pw,m}\, c_{t,m}, \tag{32}$$

where $F_{pw,m} = \dfrac{1}{\phi + \rho_o \phi_o K_{d,o,m} + \rho_i \phi_i K_{d,i,m}}$,

and

$$c_{o,m} = F_{o,m}\, c_{t,m}, \tag{33}$$

where $F_{o,m} = \dfrac{\rho_o \phi_o K_{d,o,m}}{\phi + \rho_o \phi_o K_{d,o,m} + \rho_i \phi_i K_{d,i,m}}$,

$$c_{i,m} = F_{i,m}\, c_{t,w}, \tag{34}$$

where $F_{i,m} = \dfrac{\rho_i\, \phi_i\, K_{d,i,m}}{\phi + \rho_o\, \phi_o\, K_{d,o,m} + \rho_i\, \phi_i\, K_{d,i,m}}$,

and

$$c_{d,m} = F_{d,m}\, c_{t,m}, \tag{35}$$

where $F_{d,m} = \phi F_{pw,m}$.

Thus,

$$c_{pw,m} = F_{pw,m}\, c_{t,m}, \tag{36}$$

$$c_{d,m} = \phi c_{pw,m} = F_{d,m}\, c_{t,m}, \tag{37}$$

$$\nu_{o,m} = \frac{V_{t,m}}{m_{o,m}} F_{o,m}\, c_{t,m}, \tag{38}$$

and

$$\nu_{i,m} = \frac{V_{t,m}}{m_{i,m}} F_{i,m}\, c_{t,m}. \tag{39}$$

Note that

$$F_{d,m} + F_{o,m} + F_{i,m} = 1.$$

Finally, by substituting equations (36), (37), (38), and (39) into equation (21), the total contaminant balance in the mixed sediment can be reexpressed as

$$V_{t,m} \frac{dc_{t,m}}{dt} = v_{o,w} A_w F_{o,w}\, c_{t,w} + v_{i,w} A_w F_{i,w}\, c_{t,w} - v_b A_m\, c_{t,m}$$

$$- v_r A_m c_{t,m} - k_{d,m} V_{t,m} F_{d,m} c_{t,m} - k_{o,m} V_{t,m} F_{o,m} c_{t,m}$$

$$- k_{i,m} V_{t,m} F_{i,m} c_{t,m} + \frac{\phi E_s A_m}{z_b'} \left(F_{d,w} c_{t,w} - F_{pw,m} c_{t,m}\right)$$

$$+ \frac{\phi E_s A_m}{z_{1,2}} \left(F_{pw,2} c_{t,2}^* - F_{pw,m} c_{t,m}\right). \tag{40}$$

2.1.3 Deep Sediment Balance

The total contaminant budget for the remaining segments is formulated in much the same way as that of the mixed sediment layer. The settling term is represented as a product of the settling velocity, sediment surface area, and concentration at the interface between each segment. The concentration at the interface depends on the levels in both segments, which can be approximated by

$$c_{j,k} = \alpha_{j,k} c_j + \beta_{j,k} c_k,$$

where $c_{j,k}$ = the concentration at the interface between the jth and k^{th} segment,

c_j = concentration in the jth segment,

c_k = concentration in the kth segment, and

α,β = weighting factors ($\alpha + \beta = 1$).

Presented below is the final equation for the total contaminant in segment i, where i = 2,ns (ns being the total number of segments),

$$V_{t,i} \frac{dc_{t,i}}{dt} = v_b A_m \left(\alpha_{i-1,i} c_{t,i-1} + \beta_{i-1,i} c_{t,i}\right)$$

$$- v_b A_m \left(\alpha_{i,i+1} c_{t,i} + \beta_{i,i+1} c_{t,i+1}\right)$$

---

*It will be shown in the following section that $c_{pw,2} = F_{pw,2} c_{t,2}$.

$$+ \frac{\phi\ E_s\ A_m}{z_{i-1,i}} \left(F_{pw,i-1}\ c_{t,i-1} - F_{pw,i}\ c_{t,i}\right)$$

$$+ \frac{\phi\ E_s\ A_m}{z_{i,i+1}} \left(F_{pw,i+1}\ c_{t,i+1} - F_{pw,i}\ c_{t,i}\right)$$

$$- k_{i,i}\ V_{t,i}\ F_{i,i}\ c_{t,i} - k_{o,i}\ V_{t,i}\ F_{o,i}\ c_{t,i} - k_{d,i}\ V_{t,i}\ F_{d,i}\ c_{t,i}, \quad (41)$$

where i = segment number.

The remaining terms are the same as those used in the total contaminant balance in the mixed sediment.

2.2 Solids Budget

The contaminant budget previously described relies on the knowledge of the levels of particulate matter in the water column and sediments. Therefore a solids budget is obtained that yields the concentration of organic and inorganic solids in the two regimes, as well as the rate of burial to the deep sediments.

The spatial segmentation scheme of the solids budget is somewhat different than that of the contaminant budget. The system is divided into only two well-mixed zones, the water column and the mixed sediment, with unidirectional burial to the deep sediments. It is assumed that the solids balance is at a steady state and that compaction is negligible (i.e., porosity is constant).

The inorganic solids are assumed to be strictly allochthonous, i.e., they originate outside the lake and are transported into the system via the the wind and tributary streams. The organic solids are assumed to be autochthonous; i.e., they originate within the lake via primary production.

2.2.1 Inorganic Solids

Writing mass balances for the inorganic particulate matter in the water column and mixed sediment results in the following differential equations:

$$V_{t,w} \frac{ds_{i,w}}{dt} = \underset{\text{(loading)}}{\Psi} - \underset{\text{(flushing)}}{Q\ s_{i,w}} - \underset{\text{(settling)}}{v_{i,w}\ A_w\ s_{i,w}} + \underset{\text{(resuspension)}}{v_r\ A_m\ \rho_i\ \phi_i} \quad (42)$$

and

$$V_{t,m} \frac{d(\rho_i \phi_i)}{dt} = \underset{\text{(settling)}}{v_{i\,w} A_w s_{i\,w}} - \underset{\text{(resuspension)}}{v_r A_m \rho_i \phi_i} - \underset{\text{(settling)}}{v_b A_m \rho_i \phi_i}, \tag{43}$$

where $s_{i,w}$ = concentration of inorganic suspended solids in the water column (= $m_{i,w}/V_{t,w}$), grams per cubic meter,

Ψ = loading rate of inorganic solids, grams per year, and

$\rho_i \phi_i$ = concentration of inorganic solids in the mixed sediment (= $m_{i,m}/V_{t,m}$), grams per cubic meter.

Remember that

$$\phi + \phi_o + \phi_i = 1. \tag{44}$$

2.2.2 Organic Solids

The concentration of organic solids is assumed to be directly proportional to the level of particulate organic phosphorus, as in

$$s_{o,w} = \frac{p_{o,w}}{\alpha_{pd}} \tag{45}$$

and

$$\rho_o \phi_o = \frac{p_{o,m}}{\alpha_{pd}}, \tag{46}$$

where $s_{o,w}$ = concentration of organic suspended solids in the water column (= $m_{o,w}/V_{t,w}$), grams per cubic meter,

$p_{o,w}$ = concentration of particulate organic phosphorus in the water column, milligrams of phosphorus per cubic meter,

$p_{o,m}$ = concentration of particulate organic phosphorus in the mixed sediment, milligrams of phosphorus per cubic meter,

α_{pd} = fixed stoichiometric coefficient, milligrams of phosphorus per gram, and

$PO\phi_o$ = concentration of organic solids in the mixed sediment ($= m_{o,m}/V_{t,m}$), grams per cubic meter.

A mass balance written for total phosphorus in the water column yields

$$V_{t,w}\frac{dp_{t,w}}{dt} = \underset{\text{(loading)}}{W_p} - \underset{\text{(flushing)}}{Q\,p_{t,w}} - \underset{\text{(settling)}}{v_{o,w}\,A_w\,p_{o,w}} - \underset{\text{(settling)}}{v_{i,w}\,A_w\,p_{i,w}}$$

$$+ \underset{\text{(resuspension)}}{v_r\,A_m\left(p_{o\,m} + p_{i,m}\right)}, \tag{47}$$

where $p_{t\,w}$ = total phosphorus concentration in the water column, milligrams of phosphorus per cubic meter,

W_p = rate of total phosphorus loading, milligrams of phosphorus per year,

$p_{i,w}$ = concentration of particulate inorganic phosphorus in the water column, milligrams of phosphorus per cubic meter, and

$p_{i,m}$ = concentration of particulate inorganic phosphorus in the mixed sediment, milligrams of phosphorus per cubic meter.

Note that

$$p_{t,w} = p_{d,w} + p_{o,w} + p_{i,w}, \tag{48}$$

where $p_{d,w}$ = concentration of dissolved phosphorus in the water column, milligrams of phosphorus per cubic meter.

The individual terms $p_{o,w}$ and $p_{i,w}$ can be expressed in terms of total phosphorus, $p_{t\,w}$, with the use of some conversion factors, as in

$$p_{o,w} = F_{p,o,w}\,p_{t,w}, \tag{49}$$

where $F_{p,o,w} = \dfrac{\P_o}{1 + \P_o + K_{d,i,p}\, s_{i,w}}$,

and

$$p_{i,w} = F_{p,i,w}\, p_{t,w}, \tag{50}$$

where $F_{p,i,w} = \dfrac{K_{d,i,p}\, s_{i,w}}{1 + \P_o + K_{d,i,p}\, s_{i,w}}$

The terms $\P_o$ and $K_{d,i,p}$ are partition coefficients that relate the particulate and dissolved fractions, as in

$$\P_o = \frac{p_{o,w}}{p_{d,w}}$$

and

$$K_{d,i,p} = \frac{\nu_{p,i,w}}{p_{d,w}},$$

where $\nu_{p,i,w}$ = mass specific concentration of phosphorus associated with inorganic solids, milligrams of phosphorus per gram.

Substituting equations (49) and (50) into equation (47) yields

$$V_{t,w} \frac{dp_{t,w}}{dt} = W_p - Q\, p_{t,w} - v_{o,w}\, A_w\, F_{p,o,w}\, p_{t,w} - v_{i,w}\, A_w\, F_{p,i,w}\, p_{t,w}$$

$$+ v_r\, A_m \left(p_{o,m} + p_{i,m}\right). \tag{51}$$

The mass balance equations for organic and inorganic particulate phosphorus in the mixed sediment are, respectively,

$$V_{t,m} \frac{dp_{o,m}}{dt} = \underbrace{v_{o\,w} A_w F_{p,o,w} p_{t,w}}_{\text{(settling)}} - \underbrace{v_r A_m p_{o,m}}_{\text{(resuspension)}} - \underbrace{v_b A_m p_{o,m}}_{\text{(settling)}}$$

$$- \underbrace{K_m V_{t,m} p_{o,m}}_{\text{(remineralization)}} \tag{52}$$

and

$$V_{t,m} \frac{dp_{i,m}}{dt} = \underbrace{v_{i,w} A_w F_{p,i,w} p_{t,w}}_{\text{(settling)}} - \underbrace{v_r A_m p_{i,m}}_{\text{(resuspension)}} - \underbrace{v_b A_m p_{i,m}}_{\text{(settling)}}$$

$$+ \underbrace{K_m V_{t,m} p_{o,m}}_{\text{(remineralization)}}, \tag{53}$$

where K_m = remineralization rate, per year.

Equations (42), (43), (44), (51), (52), and (53) represent six non-linear equations with six unknowns--$s_{i,w}$, ϕ_i, v_b, $p_{t,w}$, $p_{o,m}$, and $p_{i,m}$. These equations, except equation (44), can be set equal to zero (steady-state assumption) and solved simultaneously*. Once these six parameters have been determined, then equations (45) and (46) can be used to calculate $S_{o,w}$ and ϕ_o, respectively. Finally, the values for $s_{o,w}$, $s_{i,w}$, ϕ_o, ϕ_i, and v_b are made available for use by the contaminant budget.

3. MODEL USE

Numerical integration is used to solve the set of differential equations that constitute SED. Initial contaminant values at time zero are required in all segments (i.e., the water column and each sediment layer). The physical and kinetic parameters, such as the lake and contaminant data, must also be defined before the start of the simulation. The annual rates of contaminant loading W_c are read from an input file. SED is capable of estimating the loading rates for years when there are no data by linearly interpolating between years for which data exist.

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*The authors used one of the IMSL packages (subroutine ZSYSTM) available at NOAA, Great Lakes Environmental Research Laboratory.

Before integration can begin, certain model parameters must also be specified, such as the year corresponding to time zero and the number of years of simulation. It is also necessary to have a print step to determine how often during the simulation the results are to be printed (e.g., after every year). A maximum time step of integration (i.e., one that will prevent instability) is internally calculated, but the actual time step is set at a lower value to increase accuracy. A mass balance is calculated at the end of each time step as a check that mass is being conserved throughout the simulation. Complete lists of the lake, contaminant, and model parameters used in SED are presented in tables 1, 2, and 3, respectively. All of these parameters must be defined to assure proper execution.

The model output consists of the results from the solids budget, contaminant budget, initial calculations, and mass balance. To assure their accuracy, the annual contaminant loading rates and various other input parameters are also printed as output. Finally, SED draws five plots--contaminant loading versus time, total contaminant concentration in the water column versus time, total contaminant concentration in the sediments versus depth, concentration of contaminant dissolved in the pore water versus depth, and concentration of contaminant associated with the solids in the sediment versus depth. An example of the model output is presented in the following exercise.

Example. Use the parameter values used in tables 1, 2, and 3 to simulate the concentration of ^{239}Pu in the water column and sediments of Lake Michigan from 1953 to 1977.

A copy of the model output for the above simulation is presented in appendix A and the five plots are presented in figures 4 and 5. A complete listing of SED is presented in appendix B.

TABLE 1.--*Lake parameters used in the simulation of ^{239}Pu in Lake Michigan (Chapra, 1982; Chapra and Sonzogni, 1979; Bannerman et al., 1974).*

Parameter	Symbol	Value	Units
Outflow	Q	60×10^9	$m^3\ yr^{-1}$
Air/water surface area	A_s	56×10^9	m^2
Lake surface area	A_w	50×10^9	m^2
Sediment surface area	A_m	30×10^9	m^2
Lake depth	z_w	90.5	m
Sediment layer depths	z_s	*	m
Mixing zone	z_b	0.01	m
Number of segments	n_s	30	
Settling velocity of inorganic solids	$v_{i,w}$	109.5	$m\ yr^{-1}$
Settling velocity of organic solids	$v_{o,w}$	54.75	$m\ yr^{-1}$
Settling velocity to deep sediments	v_b	†	$m\ yr^{-1}$
Resuspension rate	v_r	0	$m\ yr^{-1}$
Inorganic solids concentration in the water column	$s_{i,w}$	†	$g\ m^{-3}$
Organic solids concentration in the water column	$s_{o,w}$	†	$g\ m^{-3}$
Rate of inorganic solids loading	Ψ	6×10^{12}	$g\ yr^{-1}$
Porosity	ϕ	0.8	
Ratio of inorganic solids volume to total volume in sediment	ϕ_i	†	

TABLE *1.--Lake parameters used in the simulation of ^{239}Pu in Lake Michigan-4cont.I*

Parameter	Symbol	Value	Units
Ratio of organic solids volume to total volume in sediment	ϕ_o	†	
Inorganic solids density	ρ_i	2.5×10^6	$g\ m^{-3}$
Organic solids density	ρ_o	1.27×10^6	$g\ m^{-3}$
Total phosphorus loading rate	W_p	6×10^{12}	$mgP\ yr^{-1}$
Stochiometric coefficient-organic P/dry weight	α_{pd}	10	$mgP\ g^{-1}$
Partition coefficient-inorganic P/dissolved P	$K_{d,i,p}$	0.001	$m^3\ g^{-1}$
Partition coefficient-organic P/dissolved P	π_o	0.333	
Remineralization rate of organic P to inorganic P	K_m	0.001	yr^{-1}

*The segement depths, starting from the mixed sediment, are as follows (in centimeters):

2, 20 x 0.5, 1, 2, 4, 8, 16, 32, 64, 128, 256.

†These values are internally calculated by the solids budget and then input to the contaminant budget.

TABLE 2.--*Contaminant parameters used in the simulation of ^{239}Pu in Lake Michigan (Chapra, 1982; Wahtgren et al., 1980)*

Parameter	Symbol	Value	Units
Loading rate	W_c	*	Ci yr^{-1}
Initial contaminant concentration	c_o	0	Ci m^{-3}
Molecular diffusion	E_m	1.21×10^{-5}	cm^2 s^{-1}
Vaporization rate	v_v	0	m yr^{-1}
Decay rates in water column	$k_{d,w}$, $k_{o,w}$, $k_{i,w}$	0	yr^{-1}
Decay rates in sediments	$k_{d,m}$, $k_{o,m}$, $k_{i,m}$	0	yr^{-1}
Inorganic partition coefficient in the water column	$K_{d,i,w}$	5×10^5	
Organic partition coefficient in the water column	$K_{d,o,w}$	5×10^5	
Inorganic partition coefficient in sediments	$K_{d,i,m}$	2×10^4	-
Organic partition coefficient in sediments	$K_{d,o,m}$	2×10^4	-

*See figure 4 (left).

TABLE 3.--*Model parameters used in the simulation of* ^{239}Pu *in Lake Michigan*

Parameter	Symbol	Value	Units
Year at time zero	t_o	1953	yr
Number of years of simulation	n_y	25	yr
Print step	t_p	1	yr
Time step	t_c	0.005	yr

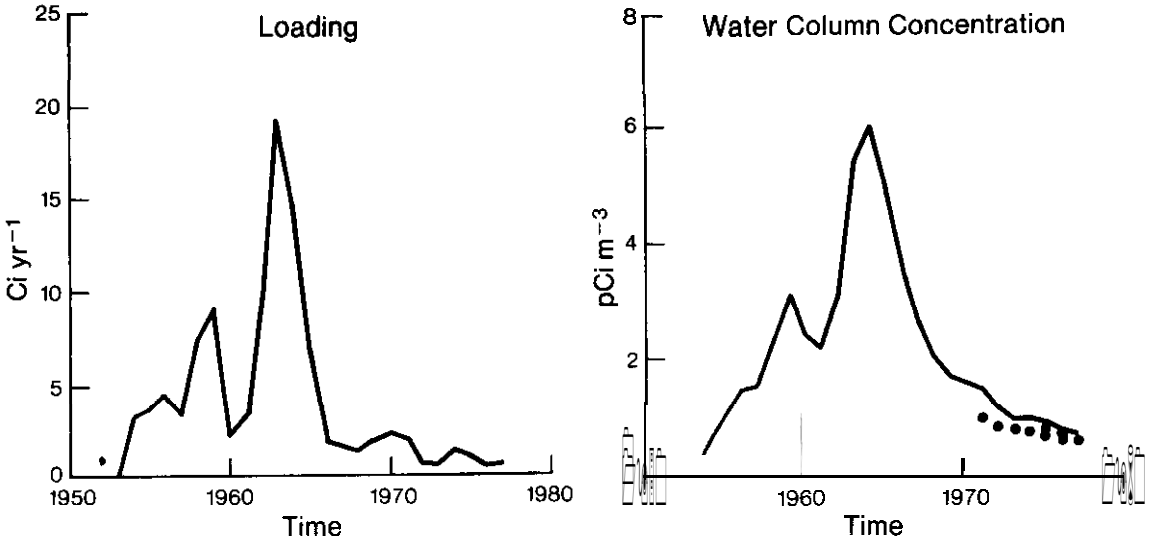

FIGURE 4.--*Loading rate* of ^{239}Pu *to Lake Michigan, 1953-77* ($Ci\ yr^{-1}$) *(left)*, and *simulated total* concentration of ^{239}Pu *in water column* ($pCi\ m^{-3}$) (right).

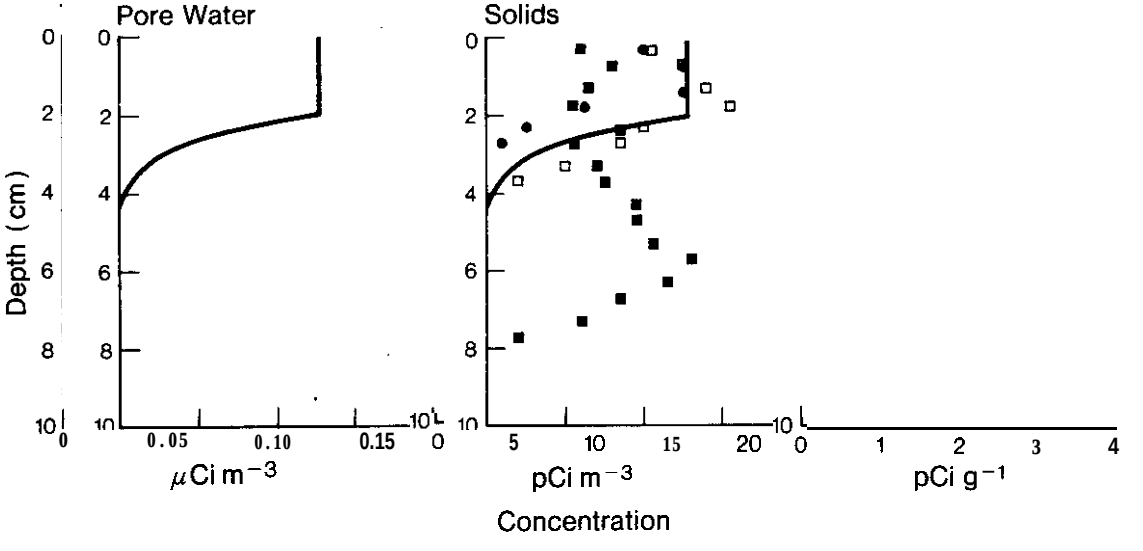

FIGURE 5.--*Simulated* total concentration of ^{239}Pu in *Lake Michigan sediments, 1973* ($\mu\ Ci\ m^{-3}$) *(left); simulated pore water concentration, 1973* ($pCi\ m^{-3}$) *(middle); simulated solids concentration, 1973* ($pCi\ g_d^{-1}$) (right).

4. REFERENCES

Bannerman, R. T., Armstrong, D. E, Holdren, G. C., and Harris, R. F. (1974): Phosphorus mobility in Lake Ontario sediments (IFYGL). In: *Proc.* ***Seventeenth*** *Conf. on Great* ***Lakes Res., Part*** *1,* International Association for Great Lakes Research, McMaster University, and Canada Centre for Inland Waters, Hamilton, Ont., August 12-14, 1974, pp. 158-178.

Chapra, S. C. (1982): Long-term models of interactions between solids and contaminants in lakes. Ph.D. dissertation. The Univ. of Mich., Ann Arbor, pp. 76-106.

Chapra, S. C., and Sonzogni, W. C. (1979): Great Lakes total phosphorus budget for the mid 1970s. *J.* ***Water Pollution Control Federation*** 51:2524-2533.

Chapra, S. C., and Reckhow, K. H. (1982): ***Engineering Approaches for*** *Lake Management--Vol.* ***2: Mechanistic Modeling.*** Ann Arbor Science, Ann Arbor, Mich., (in press).

Wahlgren, M. A., Robbins, J. A., Edgington, D. N. (1980): Plutonium in the Great Lakes. In: *Transuranic* ***Elements in the Environment,*** ed. W. C. Hanson, U.S. Department of Energy, 746 pp.

Appendix A--EXAMPLE OF MODEL OUTPUT FOR ^{239}Pu SIMULATION IN LAKE MICHIGAN

```
.....LAKEPARAMETERS-LAKE MICHIGAN.....

    Q (CU M/YR) =      .6000E+11
    AS   (SQ M)=       .5600E+11
    AW (SQ M) =        .5000E+11
    AM (SQ M) =        .3000E+11
    ZW (M) =           90.500
    VO (M/YR) =        54.750
    VI (M/YR) =       109.500
    VR (M/YR) =         0.000
    ZB (M) =             .010
    PSI (G/YR) =       .6000E+13
    WP (MG P/YR) =     .6000E+13
    KREM (/YR)  =      .0010
    KDIP (CU M/G) =   .0010
    PARA =              .3333
    APD (MP P/G)  =    10.00


.....CONTAMINANT PARAMETERS-PLUTONIUM.....

    KRW (/YR)  =            0.000
    KRS (/YR) =             0.000
    KDOW (CU M/G) =          .500
    KDIW (CU M/G)  =         .500
    KDOM (CU M/G) =          .020
    KDIM (CU M/G) =          .020
    E S (SQ M/YR)  =         .0244
    VV (M/YR) =             0.0000


     ... ..SOLIDS BUDGET......

    PTW (MG P/CU M)  =   8.0186
    POM ,MG P/CU M)  =    .3771E+06
    PIM ,MG P/CU M)  =    .1879E+05
    SIW ,G/CU M)  =      1.0840
    PHII                  .1703
    VB (M/YR) =           .4647E-03


  ......INITIALCALCULATIONS......

    SOW (G/CU M) =            .2003
    SIW (G/CU M) =           1.0840
    PHIO*RHOO (G/CU M)  =     .3771E+05
    PHII*RHOI (G/CU M)  =     .4258E+06
    FOW =            .6090E+00
    FOW =            .6099E-01
    FIW =            .3301E+00
    FPWM =           .1079E-03
    FOM =            .8630E-04
    FOM =            .8136E-01
    FIM =            .9186E+00
    PHI =            .8000
    PHIO =           .0297
    PHI, =           .1703
```

SEGMENT	SEGMENT DEPTH	ALPHA(I,I+1)	BETA(I,I+1)
1	.020	1.0000	0.0000
2	.005	.5000	.5000
3	.005		.5000
4	.005	.5000	.5000
5	.005	.5000	.5000
6	.005	.5000	.5000
7	.005	.5000	.5000
8	.005	.5000	.5000
9	.005	.5000	.5000
10	.005	.5000	.5000
11	.005	.5000	.5000
12	.005	.5000	.5000
13	.005	.5000	.5000
14	.005	.5000	.5000
15	.005	.5000	.5000
16	.005	.5000	.5000
17	.005	.5000	.5000
18	.005	.5000	.5000
19	.005	.5000	.5000
20	.005	.5000	.5000
21	.005	.6667	.3333
22	.010	.6720	.3280
23	.020	.8610	.1390
24	.040	.9555	.0445
25	.080	1.0000	0.0000
26	.160	1.0000	0.0000
27	.320	1.0000	0.0000
28	.640	1.0000	0.0000
29	1.280	1.0000	0.0000
30	2.550	1.0000	0.0000
31	5.120	1.0000	0.0000

THE TIME STEP OF INTEGRATION(YEARS)=.005

.....MASS BALANCE RESULTS(CURIES).....

TIME	INPUT	OUTPUT	DIFF	ACCUM
1977.	103.4880	3.1413	100.3467	100.3467

FLUSH	VAPOR	DECAY	SETTLE
3.1413	0.0003	0.0000	0.0000

.....LOADING (CURIES/YEAR).....

TIME	LOAD
1953.	0.00
1954.	3.36
1955.	3.75
1956.	4.48
1957.	3.42
1958.	7.56
1959.	9.24
1960.	2.24
1961.	3.42
1962.	9.52
1963.	19.15
1964.	14.56
1965.	6.16
1966.	1.85
1967.	1.68
1968.	1.40
1969.	1.96
1970.	2.41
1971.	2.13
1972.	.73
1973.	.62
1974.	1.46
1975.	1.12
1976.	.56
1977.	.73

.....CONCENTRATION IN THE WATER COLUMN.....

TIME	TOTAL CI/CU M	DISS CI/CU M	INORG CI/CU M	INORG CI/GM	ORG CI/CU M	ORG CI/GM
1953.	0.	0.	0.	0.	0.	0.
1954.	.5975E-12	.3638E-12	.1972E-12	.1819E-12	.3644E-13	.1819E-12
1955.	.1048E-11	.6379E-12	.3458E-12	.3190E-12	.6389E-13	.3190E-12
1956.	.1465E-11	.8921E-12	.4835E-12	.4461E-12	.8935E-13	.4461E-12
1957.	.1544E-11	.9402E-12	.5096E-12	.4701E-12	.9416E-13	.4701E-12
1958.	.2334E-11	.1422E-11	.7705E-12	.7108E-12	.1424E-12	.7108E-12
1959.	.3140E-11	.1912E-11	.1036E-11	.9560E-12	.1915E-12	.9560E-12
1960.	.2413E-11	.1469E-11	.7965E-12	.7347E-12	.1472E-12	.7347E-12
1961.	.2166E-11	.1319E-11	.7150E-12	.6596E-12	.1321E-12	.6596E-12
1962.	.3099E-11	.1887E-11	.1023E-11	.9437E-12	.1890E-12	.9437E-12
1963.	.5410E-11	.3295E-11	.1786E-11	.1647E-11	.3300E-12	.1647E-11
1964.	.6072E-11	.3697E-11	.2004E-11	.1849E-11	.3703E-12	.1849E-11
1965.	.5010E-11	.3051E-11	.1654E-11	.1525E-11	.3056E-12	.1525E-11
1966.	.3580E-11	.2180E-11	.1182E-11	.1090E-11	.2184E-12	.1090E-11
1967.	.2650E-11	.1614E-11	.8745E-12	.8068E-12	.1616E-12	.8068E-12
1968.	.2013E-11	.1226E-11	.6645E-12	.6130E-12	.1228E-12	.6130E-12
1969.	.1711E-11	.1042E-11	.5649E-12	.5211E-12	.1044E-12	.5211E-12
,970.	.1601E-11	.9748E-12	.5284E-12	.4874E-12	.9763E-13	.4874E-12
1971.	.1482E-11	.9024E-12	.4891E-12	.4512E-12	.9038E-13	.4512E-12
1972.	.1158E-11	.7053E-12	.3823E-12	.3527E-12	.7064E-13	.3527E-12
1973.	.9329E-12	.5681E-12	.3079E-12	.2841E-12	.5690E-13	.2841E-12
1974.	.9388E-12	.5717E-12	.3099E-12	.2858E-12	.5726E-13	.2858E-12
1975.	.8822E-12	.5372E-12	.2912E-12	.2686E-12	.5380E-13	.2686E-12
1976.	.7461E-12	.4544E-12	.2463E-12	.2272E-12	.4550E-13	.2272E-12
1977.	.6887E-12	.4194E-12	.2273E-12	.2097E-12	.4200E-13	.2097E-12

.....TOTAL CONCENTRATION IN THE SEDIMENT.....
(CURIES/CU METER)

	.0200	.0225	.0275	.0325	.0375
1973.	.1183E-06	.7777E-07	.3987E-07	.1681E-07	.6095E-08
	.0425	.0475	.0525	.0575	.0625
1973.	.1954E-08	.5635E-09	.1479E-09	.3560E-10	.7905E-11
	.0675	.0725	.0775	.0825	.0875
1973.	.1627E-11	.3117E-12	.5584E-13	.9386E-14	.1486E-14
	.0925	.0975	.1025	.1075	.1125
1973.	.2221E-15	.3145E-16	.4229E-17	.5413E-18	.6610E-19
	.1175	.1250	.1400	.1700	.2300
1973.	.7781E-20	.4304E-21	.8952E-23	.9290E-25	.4705E-27
	.3500	.5900	1.0700	2.0300	3.9500
1973.	.1149E-29	.1320E-32	.7208E-36	.1883E-39	.2363E-43
	7.7900				
1973.	.1428E-47				

.....CONCENTRATION IN THE PORE WATER.....
(CURIES/CU METER OF PORE WATER)

	.0200	.0225	.0275	.0325	.0375
1973.	.1276E-10	.8389E-11	.4300E-11	.1814E-11	.6575E-12
	.0675	.0725	.0775	.0825	.0875
1973.	.1755E-15	.3362E-16	.6023E-17	.1012E-17	.1603E-18
	.0925	.0975	.1025	.1075	.1125
1973.	.2396E-19	.3392E-20	.4561E-21	.5839E-22	.7130E-23
	.1175	.1250	.1400	.1700	.2300
1973.	.8393E-24	.4643E-25	.9657E-27	.1002E-28	.5075E-31
	.3500	.5900	1.0700	2.0300	3.9500
, 9 7 3 .	.1239E-33	.1423E-36	.7775E-40	.2032E-43	.2549E-47
	7.790"				
1973.	.1540E-51				

.....CONCENTRATION ON THE SOLIDS.....
(CURIES/GRAM OF SOLID,
ORGANIC--INORGANIC

	.0200 METERS		.0225 METERS		.0275 METERS	
1973.	.2552E-12	.2552E-12	.1678E-12	. 1678E-12	.8601E-13	.8601E-13
	.0325 METERS		.0375 METERS		.0425 "ETERS	
1973.	.3627E-13	.3627E-13	.1315E-13	.1315E-13	.4215E-14	.4215E-14
	.0475 METERS		.0525 METERS		.0575 METERS	
1973.	.1216E-14	.1216E-14	.3191E-15	.3191E-15	.7681E-16	.7681E-16
	.0625 METERS		.0675 METERS		.0725 METERS	
1973.	.1705E-16	.1705E-16	.3510E-17	.3510E-17	.6725E-18	.6725E-18
	.0775 METERS		.0825 METERS		.0875 "ETERS	
1973.	.1205E-18	.1205E-18	.2025E-19	.2025E-19	.3205E-20	.3205E-20
	.0925 METERS		.0975 METERS		.1025 METERS	
1973.	.4791E-21	.4791E-21	.6784E-22	.6784E-22	.9123E-23	.9123E-23
	.1075 METERS		.1125 METERS		.1175 METERS	
1973.	.1168E-23	. 1168E-23	.1426E-24	.1426E-24	.1679E-25	.1679E-25
	.1250 METERS		.1400 METERS		.1700 METERS	
1973.	.9285E-27	.9285E-27	.1931E-28	.1931E-28	.2004E-30	.2004E-30
	.2300 METERS		.3500 METERS		.5900 METERS	
1973.	.1015E-32	.1015E-32	.2478E-35	.2478E-35	.2847E-38	.2847E-38
	1.0700 METERS		2.0300 METERS		3.9500 METERS	
1973.	.1555E-41	.1555E-41	.4063E-45	.4063E-45	.5099E-49	.5099E-49
	7.7900 METERS					
,973.	.3080E-53	.3080E-53				

09.30.15.UELP, 0.365KLNS.

Appendix B.--LISTING OF SED

```
      PROGRAM SED(INPUT,OUTPUT,TAPE6=OUTPUT,TAPE1,TAPE2,TAPE3)
C
C*****************SEDIMENT/WATER COLUMN CONTAMINANT MODEL**************
C
C PURPOSE :
C                THE PURPOSE OF THIS PROGRAM IS TO SIMULATE THE CONCEN-
C                TRATION OF A CONTAMINANT IN THE SEDIMENTS AND OVERLYING
C                WATER COLUMN OF A NELL-MIXED LAKE BASED ON USER SUPPLIED
C                YEARLY LOADING RATES.
C
C                ITS PRINCIPAL APPLICATION WOULDBE TO PREDICT THE YEAR-
C                TO-YEAR AND STEADY-STATE RESPONSES OF THE WATER COLURN
C                AND SEDIMENTS DUE TO CHANGES IN THE AMOUNT OF CONTAHINANT
C                AND/OR PARTICULATE HATTER ENTERING THE LAKE.
C
C
C INPUT :
C   REAL UNIT 1 :
C     CONTAHINAYT LOADING RATES :
C                                                          FORMAT    COLUMN
C                TX - YEAR CORRESPONDING TO LOAD            F10.3     1-10
C                W Y - LOADING RATE IF CI/CM**2/YR)         F10.3    11-20
C
C   REAL UNIT 3 :
C     DATA POINTS FOR PLOTS :
C
C                PLTIME - YEAR                              F7.1      1-7
C                PLCDNCY - WATER COLUMN CONCENTRATION       F7.L      8-14
C                          (P CI/CU M)
C                DEPTH1 - DEPTH (CM)                        F7.1      1-7
C                PLCONC1 - TOTAL SEDIMENT CONCENTRATION     F7.1      8-14
C                          (MICRO CI/CUM)
C                DEPTH2 - DEPTH (CM)                        F7.1      1-7
C                PLCONC2 - PORE WATER CONCENTRATION         F7.1      8-14
C                          (PCI/CUM OF PORE WATER)
C                DEPTH3 - DEPTH (CM)                        F7.1      1-7
C                PLCONC3 - SDLIDS CONCENTRATION             F7.1      8-14
C                          (PCI/GM OF SOLID)
C
C
C OUTPUT :
C   REAL UNIT 6
C                LAKE PARAMETERS
C                CONTAMINANT PARAMETERS
C                SOLIDS BUDGET RESULTS
C                INITIAL CALCULATION RESULTS
C                SEGMENT, SEGMENT DEPTH, ALPHA, BETA
C                TINE STEP OF INTEGRATION
C                MASS BALANCE RESULTS
C                LOADING RATES
```

```
C                 SIMULATION RESULTS
C                     - WATER COLUMN CONCENTRATION
C                     - TOTAL SEDIMENT CONCENTRATION
C                     - PORE WATER CONCENTRATION
C                     - SOLIDS CONCENTRATION
C
C
C PLOTTING :
C   REAL UNIT 2
C                 LOADING RATE VERSES TIME
C                 WATER COLUMN CONCENTRATION VERSES TIRE
C                 TOTAL SEDIMENT CONCENTRATION VERSES DEPTH
C                 PORE WATER CONCENTRATION VERSES DEPTH
C                 SOLIDS CONCENTRATION VERSES DEPTH
C
C
C SUBROUTINES :
C                 RMAX - CALCULATES MAXIMUM VALUE FROM ARRAY OF VALUES
C                 ZSYSTM - SIMULTANEOUSLY SOLVES SET OF NON-LINEAR EQUATIONS
C                          (AVAILABLE IN IMSL SOFTWARE)
C                 FUNCTION SOLID - SUPPLIES ZSYSTM WITH SET OF NON-LINEAR
C                                  EQUATIONS
C
C
C
      INTEGER PLOTYR
      REAL KDIW,KDOW,KDIM,KDOM,KRW,KRS,NYR,KDIP,KREM,INPUT,INIT,VIW,VOW
      DIMENSION CTM(50,40),AL(40,40),TT(50)
      DIMENSION ZS(31),DCMDT(40),CM(40),CTW(50)
      DIMENSION ALPHA(40,40),BETA(40,40)
      DIMENSION Z(40,40),VM(40),TIME(50),WC(50)
      DIMENSION CDW(50),CIW(50),COW(50),VOW(50),VIW(50),CPWM(50,40)
      OIMENSION ZYY(40),CTMX(40),CPWMX(40),VOMX(40),VIMX(40)
      DINENSION CMAX(2),CTWX(50),ZYYY(40),CMDK(50)
      DIMENSION TX(50),TTX(50),WW(50),VOM(40,40),VIM(40,40)
      DIMENSION PLTIME(10),PLCONCW(10),DEPTH1(9),DEPTH2(7),DEPTH3(17)
      DIMENSION PLCONC1(9),PLCONC2(7),PLCONC3(17)
      DIMENSION X(6),WA(38),PAR(16),IPAK(30)
      EXTERNAL SOLID
C
C
C SEGMENT LENGTHS (CM)
      DATA ZS/2.,20*.5,1.,2.,4.,8.,16.,32.,64.,128.,256./
C
C
C LAKE PARAMETERS--LAKE MICHIGAN
      ZW=90.5
      AW=50000.0E6
      AS=56000.0E6
      Q=60.0E9
      VI-.3*365.
      vo-.15*365.
      VR-0.0
      AM=30000.0E6
      ZB=1./100.
      PHI=.80
      RHOO=1.27E6
      RHOI=2.5E6
      PSI=6.0E12
      WP=6.0E12
```

```
      KREM=.001
      KDIP=.001
      PARA=.33333
      APD=10.
C
      VTW=AW*ZW
      VTM=AM*ZS(1)/100.
C
C
C  MODEL PARAMETERS
C   NUMBER OF SEGMENTS (MULTIPLES OF TEN ARE BEST FOR OUTPUT)
      NS-30
C
C   PRINT STEP
      TP-1.
C
C   TIME STEP
      TC-. 005
C
C   NUMBER OF YEARS OF SIMULATION
      NYR-25.
C
C   YEAR AT TIRE ZERO
      TIME(1)=1953.
C
C
C  CONTAMINANT  PARAMETERS--PLUTONIUM
C   DECAY RATES
      KRW=0.
      KRS=0.
C
C   PARTITION COEFFICIENTS
      KDIW=5.0E5
      KDOW=5.0E5
      KDIM=2.0E4
      KDOM=2.0E4
C
C   DIFFUSION COEFFICIENT
      EM=1.21E-5
      ES=EM*PHI**2
C
C   VAPORIZATION RATE
      vv-0.0
C
C   INITIAL  CONCENTRATIONS
      CW=0.
      CTW(1)=CW
      DO 10 I=1,NS
       CM(I)=0.
       CTM(1,I)=CM(I)
   10 CONTINUE
      CM(NS+1)=CM(NS)
C
C
C  LOADING
      CONY-I.0
      DO 30I=1,99
       READ(1,1010)TX(I),WW(I)
       IF(EOF(1))40.20
C   CONVERT FCI/CM**2/YR TO CI/YR
```

```
   2  0 WW(I)=WW(I)*1.0E-15*AS*100**2/CONV
   30 CONTINUE
C   INTERPOLATE FOR NO-LOAD YEARS
   40 TTX(1)=TX(1)
      WC(1)=WW(1)
      I=2
      NY-NYR
      DO 60 J=2,NY
       TTX(J)=TTX(J-1)+TP
       IF(TTX(J).LE.TX(I))GO TO 50
       I=I+1
   50  WC(J)=WW(I-1)+(WW(I)-WW(I-1))/(TX(I)-TX(I-1))*(TTX(J)-TX(I-1))
   60 CONTINUE
C
C
C  CONVERSIONS
      ES=ES*60.*60.*24.*365./(100.*100.)
      KDIW=KDIW/1.0E6
      KDOW=KDOW/1.0E6
      KDIM=KDIM/1.0E6
      KDOM=KDOM/1.0E6
C
      DO 70 I=1,NS
       ZS(I)=ZS(I)/100.
   70 CONTINUE
      ZS(NS+1)=ZS(NS)
C
C
C   PRINT LAKE PARAMETERS
      WRITE(6,1020)Q,AS,AW,AM,ZW,VO,VI,VR,ZB,PSI,WP,KREM,KDIP,PARA,APD
C
C   PRINT CONTAMINANT PARAMETERS
      WRITE(6,1030)KRW,KRS,KDOW,KDIW,KDOM,KDIM,ES,VV
C
C
C  SOLIDS BUDGET
      PAR(1)=PSI     $PAR(2)=Q       $PAR(3)=VI      $PAR(4)=AW
      PAR(5)=VR      $PAR(6)=AM      $PAR(7)=RHOI    $PAR(8)=PHI
      PAR(9)=APD     $PAR(10)=RHOO   $PAR(11)=WP     $PAR(12)=VO
      PAR(13)=PARA   $PAR(14)=KDIP   $PAR(15)=KREM   $PAR(16)=VTM
C
C   ZSYSTM PARAMETERS
      EPS=1.0E-6
      NSIG=6
      ITMAX=10
      N-b
      X(1)-377100.
      X(2)=18790.
      X(3)=8.0186
      X(4)=1.0840
      X(51-.1703
      X(6)=.4647E-3
C
      CALL ZSYSTM(SOLID,EPS,NSIG,N,X,ITMAX,WA,PAR,IER)
C
      POM=X(1)
      PIM=X(2)
      PTW=X(3)
      SIW=X(4)
      PHII=X(5)
```

```
      VB=X(6)
C
C   PRINT SOLIDS BUDGET RESULTS
      WRITE(6,1040)PTW,POM,PIM,SIW,PHII,VB
C
      PHIO=POM/(APO*RHOO)
      SIM=RHOI*PHII
      SOM=RHOO*PHIO
      SOW=PARA/(1.+PARA+KDIP*SIW)*PTW/APD
      FIW=KDIW*SIW/(1.+KDIW*SIW+KDOW*SOW)
      FOW=KDOW*SOW/(1.+KDIW*SIW+KDOW*SOW)
      FDW=(1.-FOW-FIW)
      FPWM=1.0/(PHI+PHII*RHOI*KDIM+PHIO*RHOO*KDOM)
      FDM=PHI*FPWM
      FOM=KDOM*RHOO*PHIO/(PHI+KDIM*RHOI*PHII+KDOM*RHOO*PHIO)
      FIM=KDIM*RHOI*PHII/(PHI+KDIM*RHOI*PHII+KDOM*RHOO*PHIO)
C
C
C INITIAL CALCULATIONS
C   MID-SEGMENT LENGTHS
      ZYY(1)=ZS(1)
      ZYY(2)=ZS(1)+ZS(2)/2.
C   ZYY(1)=ZS(1) BECAUSE 1ST SEG IS COMPLETELY MIXED
      DO 80 I=3,NS
       ZYY(I)=ZYY(I-1)+ZS(I-1)/2.+ZS(I)/2.
   80 CONTINUE
C
C   CALCULATION OF VM,Z,ALPHA AND BETA
      DO 150 I=1,NS
       VM(I)=AM*ZS(I)
       ZYYY(I+1)=ZYY(I)*100.
       ZYYY(1)=0.
       Z(I,I+1)=(ZS(I)+ZS(I+1))/2.
       AL(I,I+1)=ZS(I+1)/(ZS(I)+ZS(I+1))
       ALPHA(I,I+1)=1.05-ES*FPWM/(Z(I,I+1)*VB)
       IF(ALPHA(I,I+1).LE.1.0)G OTO120
       ALPHA(I,I+1)=1.0
       GO TO 140
  120  IF(ALPHA(I,I+1).GT.AL(I,I+1))CD TO 130
       ALPHA(I,I+1)=AL(I,I+1)
  130  IF(ALPHA(I,I+1).GE.0.5)GO TO 140
       ALPHA(I,I+1)=0.5
  140  BETA(I,I+1)=1.-ALPHA(I,I+1)
  150 CONTINUE
      ALPHA(1,2)=1.0
      BETA(1,2)=1.-ALPHA(1,2)
C
C
C
C   PRINT INITIAL CALCULATION RESULTS
      WRITE(6,1050)SOW,SIW,SOM,SIM,FDW,FOW,FIW,FPWM,FDM,FOM,FIM,PHI,PHIO
     *,PHI I
C
C
C   PRINT SEGMENT LENGTHS AND WEIGHTING FACTORS
      NRITE16.10601
      WRITE(6,1070)(I,ZS(I),ALPHA(I,I+1),BETA(I,I+1),I=1,NS)
C
C
C   CALCULATION OF TIME STEP
```

```
      DO 170 I=1,NS
       TT(I)=1./(2.*(ES*FPWM)/Z(I,I+1)**2+KRS-VB/Z(I,I+1)*(BETA(I,I+1)-A
     • LPHA(I,I+1)))
       IF(I.GT.1) GO TO160
       TMIN=TT(1)
  160  IF(TMIN.LE.TT(I))GO TO 170
       TMIN=TT(I)
  170 CONTINUE
      TCC=TMIN
      NCC=TP/TCC
      NCC=NCC+1
      TCC=TP/NCC
      IF(TCC.GT.TC)G O  T O180
      TC-TCC
C
C   PRINT TIME STEP OF INTEGRATION
  180 WRITE(6,1080)TC
C
C   INITIAL MASS
      CMTI-O.
      DO 190 I=1,NS
       CMTI=CMTI+CM(I)*VM(I)
  190 CONTINUE
      INIT=CW*VTW+CMTI
C
      INPUT-O.
      OUTPUT-O.
      FLUSH-O.
      VAPOR-O.
      DECAY-O.
      SETTLE-O.
C
C   PRINT HEADING FOR BASS BALANCE RESULTS
      WRITE(6,1090)
C
C
      NP=NYR/TP+.000001
      NC=TP/TC+.000001
C
C
C
C START OF INTEGRATION
      DO 270 J=1,NP
       DO 250 K=1,NC
C
        IF(J.EQ.1) GO TO ZOO
        TIME(J)=TIME(J-1)+TP
C
C
C   WATER COLUMN BALANCE
  200   CWLD=WC(J)
        CWFL=Q*CW*(-1.)
        CWVV=VV*AS*FDW*CW*(-1.)
        CWOS=VO*AW*FOW*CW*(-1.)
        CWIS=VI*AW*FIW*CW*(-1.)
        CWRE=VR*AM*CM(1)
        CWDB=ES*AM/((ZB+ZS(1))/2.)*(PHI*FPWM*CM(1)-FDW*CW)
        CWDB=PHI*ES*AM/((ZB+ZS(1))/2.)*(FPWM*CM(1)-FDW*CW)
        CWDK=KRW*VTW*CW*(-1.)
        DCWDT=(CWLD+CWFL+CWVV+CWOS+CWIS+CWRE+CWDB+CWDK)/VTW
```

```
C
C
C    MIXED SEDIMENT LAYER BALANCE
         CMOS=CWOS*(-1.)
         CMIS=CWIS*(-1.)
         CMRE=CWRE*(-1.)
         CMSL=VB*AM*(ALPHA(1,2)*CM(1)+BETA(1,2)*CM(2))*(-1.)
         CMDU=CWDB*(-1.)
         CMDB=PHI*ES*AM/Z(1,2)*(FPWM*CM(2)-FPWM*CM(1))
         CMDK(1)=KRS*VM(1)*CM(1)*(-1.)
         DCMDT(1)=(CMOS+CMIS+CMRE+CMSL+CMDU+CMDB+CMDK(1))/VM(1)
C
C
C    REMAINING SEDIMENT LAYERS BALANCE
         DO 210 I=2,NS
          CMSG=CMSL*(-1.)
          CMSL=VB*AM*(ALPHA(I,I+1)*CM(I)+BETA(I,I+1)*CM(I+1))*(-1.)
          CMDU=CMDB*(-1.)
          CMDB=PHI*ES*AM/Z(I,I+1)*FPWM*(CM(I+1)-CM(I))
          CMDK(I)=KRS*VM(I)*CM(I)*(-1.)
          DCMDT(I)=(CMSG+CMSL+CMDU+CMDB+CMDK(I))/VM(I)
  210    CONTINUE
C
C
C MASS BALANCE
C    LOADING
         INPUT=INPUT+CWLD*TC
C
C    LOSSES
         CDKI=0.
         D  O 220 I=1,NS
          CDKI=CDKI+CMDK(I)
  220    CONTINUE
         OUTPUT=OUTPUT-(CWFL+CWVV+CWDK+CDKI+CMSL)*TC
C
C
         FLUSH=FLUSH-CWFL*TC
         VAPOR=VAPOR-CWVV*TC
         DECAY=DECAY-(CWDK+CDKI)*TC
         SETTLE=SETTLE-CMS_*TC
C
C
C
C   INTEGRATION
         CW=CW+DCWDT*TC
         DO 2 3 0 I=1,NS
          CM(I)=CM(I)+DCMDT(I)*TC
  230    CONTINUE
C
C    ACCUMULATION
         CMTI=0.
         DO 240 I=1,NS
          CMTI=CMTI+CM(I)*VM(I)
  240    CONTINUE
         ACC=(CW*VTW+CMTI)-INIT
C
  250 CONTINUE
C
        CTW(J)=CW
        CDW(J)=FDW*CW
```

```
      COW(J)=FOW*CW
      CIW(J)=FIW*CW
      VOW(J)=COW(J)/SOW
      VIW(J)=CIW(J)/SIW
      CTWX(J)=CTW(J)/1.0E-12
      DO 260 I=1,NS
       CTM(J,I)=CM(I)
       CPWM(J,I)=FPWM*CM(I)
       VOM(J,I)=FOM*CM(I)/(PHIO*RHOO)
       VIM(J,I)=FIM*CM(I)/(PHII*RHOI)
C
       IF(J.LT.NP)GO TO 260
C PLOTYR = YEAR THAT SEDIBENT RESULTS ARE TO BE PLOTTED
      PLOTYR-1973
      PLOTYR=PLOTYR-TIME(1)+1
       CTMX(I+1)=CTM(PLOTYR,I)/1.0E-6
       CPWMX(I+1)=CPWM(PLOTYR,I)/1.0E-12
       VOMX(I+1)=VOM(PLOTYR,I)/1.0E-12
       VIMX(I+1)=VIM(PLOTYR,I)/1.0E-12
  260 CONTINUE
      CTMX(1)=CTMX(2)
      CPWMX(1)=CPWMX(2)
      VOMX(1)=VOMX(2)
      VIMX(1)=VIMX(2)
C
C
  270 CONTINUE
C
C
C   PRINT MASS BALANCE RESULTS
      OFF- INPUT-OUTPUT
      WRITE(6,1100)TIME(NP),INPUT,OUTPUT,DFF,ACC,FLUSH,VAPOR,DECAY,SETTL
     *E
C
C
C   PRINT CONTAMINANT BUDGET RESULTS
C   WATER COLUMN
      WRITE(6,1110)
      WRITE(6,1120)(TIME(J),WC(J),J=1,NP)
      WRITE(6,1130)
      WRITE(6,1140)(TIME(J),CTW(J),CDW(J),CIW(J),VIW(J),COW(J),VOW(J),J=
     *1,NP)
C
C
C   TOTAL SEDIMENT
      WRITE(6,1150)
      DO 290 K=1,NS,10
       M=K+9
       IF(M.LE.NS)GO TO 280
       M=NS
  280  WRITE(6,1160)(ZYY(I),I=K,M)
       WRITE(6,1170)(TIME(J),(CTM(J,I),I=K,M),J=PLOTYR,PLOTYR)
       WRITE(6,1180)
  290 CONTINUE
C
C
C   PORE WATER
      WRITE(6,1190)
      DO 310 K=1,NS,10
       M=K+9
```

```
      IF(M.LE.NS)GO TO 300
      M=NS
  300 WRITE(6,1160)(ZYY(I),I=K,M)
      WRITE(6,1170)(TIME(J),(CPWM(J,I),I=K,M),J=PLOTYR,PLOTYR)
      WRITE(6,1180)
  310 CONTINUE
C
C
C    SOLIDS
      WRITE(6,1200)
      DO 330 K=1,NS,5
      M=K+4
      IF(M.LE.NS)GO TO 320
      M=NS
  320 WRITE(6,1210)(ZYY(I),I=K,M)
      WRITE(6,1220)(TIME(J),(VOM(J,I),VIM(J,I),I=K,M),J=PLOTYR,PLOTYR)
  330 CONTINUE
C
C
C
C
C
C PLOT RESULTS
      CALL RMAX(CTWX,NP,CWMAX)
      CALL RMAX(WC,NP,CLMAX)
      CALL RMAX(CTMX,NS,CMMAX)
      CALL RMAX(CPWMX,NS,CPWMMAX)
      CALL RMAX(VOMX,NS,VOMMAX)
      CMAX(1)=VOMMAX
      CALL RMAX(VIMX,NS,VIMMAX)
      CMAX(2)=VIMMAX
      CALL RMAX(CMAX,2,CSMAX)
      CSMAX=CSMAX/1.25
C
      READ(3,1230) (PLTIME(I),PLCONCW(I),I=1,9)
      READ(3,1230) (DEPTH1(I),PLCONC1(I),I=1,8)
      READ(3,1230) (DEPTH2(I),PLCONC2(I),I=1,6)
      READ(3,1230) (DEPTH3(I),PLCONC3(I),I=1,16)
C
C
      CALL ID("LANG",4)
      CALL TEKTRN("AUTOHC=YES,BAUD=2400,BATCH,CENTER,TERM=4014,END$",100
     *)
      CALL BGNPL(1)
      CALL NOBROR
      CALL PHYSOR(1.0,1.0)
      CALL TITLE("LOADING$",-100,"TIME",4,"CURIES/YEAR$",100,4.,4.)
      CALL MESSAG("LAKE MICHIGAN--PLUTONIUM$",100,3.0,5.5)
      CALL XTICKS(2)
      CALL XINTAX
      CALL GRAF(1950.,10.,1980.,0.,"SCALE",CLMAX)
      CALL FRAME
      CALL CURVE(TIME,WC,NP,0)
      CALL ENDGR(1)
      CALL PHYSOR(6.0,1.0)
      CALL TITLE("WATER COLUMN CONC$",100,"TIME",4,"E-12 CURIES/CU M$",1
     *00,4.,4.)
      CALL GRAF(1950.,10.,1980.,0.,"SCALE",CWMAX)
      CALL FRAME
      CALL MARKER(2)
```

```
      CALL CURVE(PLTIME,PLCONCW,9,-1)
      CALL CURVE(TIME,CTWX,NP,0)
      CALL ENDGR(2)
      CALL ENDPL(0)
C
      CALL BGNPL(2)
      CALL NOBRDR
      CALL RESET("XINTAX")
      CALL PAGE(8.5,13.0)
      CALL PHYSOR(.6r1.251
      CALL TITLE("TOTAL CONC",-10,"E-6 CURIES/CU M$",100,"DEPTH (CM)$",1
     ●  00,3.5,4.5J
      CALL MESSAG("LAKEMICHIGAN--PLUTONIUM   1973$",100,4.18,6.0)
      CALL GRAF(0.,"SCALE",CMMAX,10.,2.,0.)
      CALL FRARE
      CALL CURVE(CTMX,ZYYY,16,0)
      CALL ENDGR(1)
      CALL PHYSOR(4.7,1.25)
      CALL TITLE("PORE WATER CONC",15,"E-12CURIES/CUM O FPW$",100,"",
     *1,3.5,4.5)
      CALL GRAF(0.,"SCALE",CPWMMAX,10.,2.,0.)
      CALL FRAME
      CALL CURVE(CPWMX,ZYYY,16,0)
      CALL ENDGR(2)
      CALL PHYSOR(8.8,1.25)
      CALL TITLE("SOLIDS CONC",11,"E-12 CURIES/GM OF SOLID$",100," ",1,3
     ●  .5.4.51
      CALL GRAF(0.,"SCALE",CSMAX,10.,2.,0.)
      CALL FRARE
      CALL LINESP(2.I
      CALL LINES(" ORGANIC$",IPAK,1)
      CALL LINES("INORGANIC$",IPAK,2)
      CALL LECLIN
      CALL CURVE(VOMX,ZYYY,16,0)
      CALL DASH
      CALL CURVE(VIMX,ZYYY,16,0)
      CALL RESET("DASH")
      CALL LEGEND(IPAK,2,1.5,.35)
      CALL SCLPIC(1.2)
      CALL MARKER(0)
      CALL CURVE(PLCONC1,DEPTH1,8,-1)
      CALL MARKER(2I
      CALL CURVE(PLCONC2,DEPTH2,6,-1)
      CALL SCLPIC(.5)
      CALL MARKER(3)
      CALL CURVE(PLCONC3,DEPTH3,16,-1)
      CALL ENDGR(3)
      CALL ENDPL(0)
      CALL DONEPL
  999 STOP

C FORMAT STATERENTS
 1010 FORMAT(2F10.3)
 1020 FORMAT("1",///" .....LAKE PARARETERS-LAKE MICHIGAN....."//5X,"Q(C
     *U M/YR) =",E13.4/5X,"AS(SQ R I =",E15.4/5X,"AW  (SQ M)=",E15.4/5X,
     *"AM(SQ H I =",E15.4/5X,"ZW (M) =",F15.3/5X,"VO (M/YR) =",F12.3/5X,
     *"VI (M/YR) =",F12.3/5X,"VR (M/YR) =",F12.3/5X,"ZB (M) =",F15.3/5X,
     *"PSI (G/YR) =",E14.4/5X,"WP (MG P/YR) =",E12.4/5X,"KREM (/YR) =",F
     *10.4/5X,"KDIP (CU M/G) =",F7.4/5X,"PARA =",F17.4,/5X,"APD (MP P/G)
     * =",F8.2//)
```

```
1 0 3 0 FORMAT("0",". . . . .CONTAMINANT PARAMETERS-PLUTONIUM.....".//5X,"KRW
    *(/YR) =",F15.3/5X,"KRS (/YR) =",F15.3/5X,"KDOW (CU M/G) =",F11.3/5
    ●  X,"KDIU (CUM/G) =",F11.3/5X,"KDOM (CU M/G) =",F11.3/5X,"KDIM (CU
    *R/C) =",F11.3/5X,"ES  (SQ M/YR) =",F13.4/5X,"VV (M/YR) =",F16.4///)
1 0 4 0 FORMAT("      . . . . ..SOLIDS BUDGET......".//5X,"PTW (MG P/CU M) =",F
    *8.4/5X,"POM (MG P/CU M) =",E12.4/5X,"PIM  (MG P/CU M) =",E12.4/5X,"
    *SIW (G/CU M) =",F11.4/5X,"PHII =",F19.4/5X,"VB (M/YR) =",E18.4///)
1 0 5 0 FORMAT(/"    . . . . ..INITIAL CALCULATIONS......".//5X,"SOW (G/CU M) =
    *",F15.4/5X,"SIW(G/CU N  J =",F15.4/5X,"PHIO*RHOO (G/CU M) =",E13.4/
    *5X,"PHII*RHOI (G/CU  HI  =",E13.4/5X,"FDW =",E19.4/5X,"FOW =",E19.4/
    ●  5X+"FIn =",E19.4/5X,"FPWM =",E18.4/5X,"FDM =",E19.4/5X,"FOM =",E19
    ●  .4/5X+"FIR  =",E19.4/5X,"PHI =",F15.4/5X,"PHIO =",F14.4/5X,"PHII ="
    *,F14.4///)
1060  FORMAT(//6X,"SEGMENT",6X,"SEGMENT DEPTH",3X,"ALPHA(I,I+1)",4X,"BET
    *A(I,I+1)"//)
1 0 7 0 FORMAT(7X,I3,7X,F10.3,11X,F6.4,9X,F6.4)
1080 FORMAT(///5X,"THE TIRE STEP OF INTEGRATION (YEARS)=",F5.3//)
1 0 9 0 FORMAT("0",///36X,"..........MASS BALANCE RESULTS (CURIES).....","
    *....."//3X,"TIME",7X,"INPUT",8X,"OUTPUT",7X,"DIFF",9X,"ACCUM",16X,
    *"FLUSH",8X,"VAPOR",8X,"DECAY",8X,"SETTLE"/)
1100  FORMAT(2X,F5.0,4F13.4,8X,4F13.4)
1110  FORMAT("1",////9X,"............LOADING(CURIES/YEAR).......","..
    *."//22X,"TIME",12X,"LOAD"/)
1120  FORMAT(21X,F5.0,9X,F7.2)
1 1 3 0 FORMAT("1",////35X,"................CONCENTRATION IN THE WATER ",
    *"COLUMN . . . . . . . . . . . . . . . . .."///23X,"TIME",11X,"TOTAL",9X,"DISS",10X,"
    *INORG",7X,"INORG",10X,"ORG",9X,"ORG"/37X,"CI/CU M",7X,"CI/CU M",7X
    *,"CI/CU M",6X,"CI/GM",8X,"CI/CU M",6X,"CI/GM"/)
1140 FORMAT(22X,F5.0,8X,E10.4,4X,E10.4,4X,E10.4,2X,E10.4,4X,E10.4,2X,E1
    *0.4)
1150  FORMAT("1",///17X,".....TOTAL CONCENTRATION ","IN
    *T  H  E SEDIMENT(CURIES/CU METER)....."//)
1160  FORMAT(6X,10F12.4/)
1170  FORMAT(1X,F5.0,2X,10E12.4)
1180  FORMAT("0")
1190 FORMAT("1",///20X,"..................CONCENTRATION IN THE PORE","
    ●  UATER (CURIES/CU METER OF PORE WATER)....."//)
1200 FORMAT("1",///20X,"..................CONCENTRATION ON THE  ","SOLID
    ●  S(CURIES/GRAM OF SOLID)....."/55X,"(ORGANIC--INORGAN
    *IC)"/)
1210  FORMAT(///12X,F7.4," METERS",4(10X,F7.4," METERS")/)
1220  FORMAT(F6.0,2X,2E11.4,2X,2E11.4,2X,2E11.4,2X,2E11.4,2X,2E11.4)
1230  FORMAT(2F7.1)
      END
```

```
C
C
C
      FUNCTION SOLID(X,K,PAR)
      DIMENSION X(6) ,PAR(16)
      GO TO(10,20,30,40,50,60),K
C
   10 SOLID=PAR(1)-PAR(2)*X(4)-PAR(3)*PAR(4)*X(4)+PAR(5)*PAR(6)*X(5)*PAR
     ● 17J
      RETURN
   2 0 SOLID=PAR(3)*PAR(4)*X(4)-(PAR(5)+X(6))*PAR(6)*X(5)*PAR(7)
      RETURN
   3 0 SOLID=PAR(8)+X(5)+X(1)/(PAR(9)*PAR(10))-1.
      RETURN
   4 0 SOLID=PAR(11)-PAR(2)*X(3)-PAR(12)*PAR(13)/(1.+PAR(13)+PAR(14)*X(4)
     *)*PAR(4)*X(3)-PAR(3)*PAR(14)*X(4)/(1.+PAR(13)+PAR(14)*X(4))*PAR(4)
     **X(3)+PAR(5)*PAR(6)*(X(1)+X(2))
      RETURN
   50 SOLID=PAR(12)*PAR(13)/(1.+PAR(13)+PAR(14)*X(4))*PAR(4)*X(3)-(PAR(5
     ●     I+XI6JI+PARI6I*XI1J-PARII5J*PARII6J*XIIJ
      RETURN
   60 SOLID=PAR(3)*PAR(14)*X(4)/(1.+PAR(13)+PAR(14)*X(4))*PAR(4)*X(3)-(P
     *AR(5)+X(6))*PAR(6)*X(2)+PAR(15)*PAR(16)*X(1)
      RETURN
      END


C
C
C
      SUBROUTINE RMAX(ARRAY,NNN,AMAX)
      DIMENSION ARRAY(70)
      AMAX=ARRAY(1)
      0 0  1 0 I=2,NNN
       IF(AMAX.GT.ARRAY(I))GO TO 10
       AMAX=ARRAY(I)
   10 CONTINUE
      AMAX=AMAX*1.25
      RETURN
      END
```