RADIOACTIVITY TRANSPORT IN WATER—— MATHEMATICAL SIMULATION

Technical Report-~19

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SUMMARY

*^A*mathematical model has been developed for routing ^aradionuclide through ^amodel river system. The capabilities of this simulation model include the following characteristics:

- 1. It distributes radionuclide activity by advective and dispersional mechanisms along the longitudinal axis of the system *.*
- 2. It may be discretized into any number of segments (vertical planes normal to the longitudinal axis) as may be appropriate to describe spatial variations in radionuclide activity.
- 3 *,* It is capable of treating instantaneous, continuous, or time-varying releases of radionuclide activity.
- 4, It provides for ^atemporal description of radionuclide activity throughout the system,
- 5 **c** It provides for sorption and desorption by both plants and bottom sediments *a*

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 $\tilde{\vec{a}}$

 \bar{z}_2

 \bar{z}

 $\frac{1}{\sqrt{2}}\sum_{i=1}^{N} \frac{1}{\sqrt{2}}$

 \bar{z}

 $\frac{1}{2}$

i v

INTRODUCTION

There is increasing concern about the movement of radioactive materials in rivers, lakes and oceans since these materials can be trans ported and may be concentrated by sediments and biota. With the continued growth of the nuclear power industry, it is essential to estimate the movement of waste products . These wastes or radionuclides may enter a stream either ^a ^s soluble or relatively insoluble materials and can be transported downstream during which time either dilution or possible concentration occurs .

Once in the stream, complex physical and chemical reactions occur. The radionuclides may undergo changes in state, remain in solution, or interact with various components of the aquatic system. The more impor= tant factors that influence the concentration of radionuclides are:

- (1) the sorption of each radionuclide by bed sediments;
- _(2) the sorption of each radionuclide by aquatic plants;
- (3) the desorption of radionuclides into flowing water;
- (4) the migration of radionuclides through the bed sediments;
- (5) the movement of sediment and attached radionuclides through the normal movement of suspended sediment or bed sediments;
- (6) the period of contact and retention in the system, $i.e.,$ transport time associated with advection and dispersion.

A more comprehensive description of the factors that influence the transport of radionuclides is given by Gloyna and Ledbetter (1969).

Transport time is a function of many factors. For a given amount of radionuclides, the mode of release (constant, instantaneous, or varying), the receiving water (lake, river, etc.), and the hydraulics of the receiving water ultimately determine the dilution or reconcentration and exposure time to the ecosystem. Thus , considerable attention must be given to hydraulic

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dispersion and convection in any study dealing with the transport of radioactive
materials through an aquatic system**.**

The physical and chemical changes that occur in typical stream environ ments have been measured, and while considerable attention has been directed to finding solutions to the phenomena of hydraulic dispersion and convection, bottom sediment transport, sorption and desorption by the aquatic ecosystem, etc., the development of a general transport equation including all of these factors has yet to be undertaken.

 \bar{z}

 \overline{a}

OBJECTIVE AND **SCOPE**

Recognizing the need for a model to include interaction between the numerous factors mentioned above, the primary objective of this study was the development of a general mathematical model, in a form suitable for simulation on a digital computer, for routing a radionuclide through a model river (flume). ^A ^s a necessary part of the development of this model it was also kept in mind that the model would eventually be applied to an actual river system; however, this study was restricted to flume data. To develop this model, several general requirements must be fulfilled. These are essential to the mechanics employed in the model and are necessary for describing the overall structure of the model and for assuring the practicality and utility of the model. This model must have the following basic capabilities:

- (l) to treat advective and dispersional transfers of radionuclides along the longitudinal axis of a one-dimensional channel;
- (2) to allow the channel to be discretized into elements of uniform length and cross~section (vertical planes normal to the longitudinal axis;
- (3) to be capable of receiving instantaneous, continuous, or varying releases of radionuclides;
- (4) to provide for a temporal description of the radionuclide activity throughout the system; and
- (5) to be capable of treating the following as sources and/or sinks —
	- (a) sorption and desorption by bottom sediments, and
	- (b) sorption and desorption by aquatic plants.

PROCEDURAL DETAILS

Verification of the mathematical model was conducted in three phases. The first phase involved verifying the dispersion characteristics of the flume using dye—release data taken by Armstrong and Gloyna (1968) , The second phase incorporated sorption and desorption of radionuclides by bottom sedi-*-* ments into the model. The data used in this phase is described by Shih and Gloyna (1967). The final phase was concerned with the inclusion of sorption and desorption by aquatic plants into the model, using data given by Armstrong and Gloyna (1968). Both of the above used ^{ov}Sr as the radionuclide. All of
the above data are described in Appendix A.

FORMULATION OF THE PROBLEM

Transport

The development of transport theory is, at this time, fairly well understood and is adequately documented in the literature(Fischer, 1966; Thackston and Krenkel, 1966).

Radionuclides, in tracer amounts, are transported in a moving fluid stream by turbulent and molecular diffusion and by differential transport. The combined effects of turbulent diffusion and differential transport are called dispersion. Molecular diffusion is usually considered negligible in relation to dispersion.

The basic transport equation can be written for a three dimensional system as:

$$
\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left(D_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left(D_y \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left(D_z \frac{\partial C}{\partial z} \right) - u \frac{\partial C}{\partial x} - v \frac{\partial C}{\partial y} - w \frac{\partial C}{\partial z}
$$
(1)

where

 $C =$ concentration at any point (x, y, z) C = concentration at any point (x, y, z)
 D_x , D_y and D_z = coefficients of dispersion in the x, y, and

z directions respectively $t = time$ u, v, and w = fluid velocities in each of the coordinate directions.

In Eq. (1), term (I) represents the temporal change in concentration, term (II) represents the transport by dispersion, and term (III) represents the mass transport by convection in the longitudinal, lateral, and vertical directions, respectively. The above equation in its complete form is almost impossible to solve, even with today's high-speed computers; however, by simplifying Eq. (1) in situations where some of the terms can be neglected, solutions can be obtained.

Taylor (1954) found that for a one-dimensional system, concentration curves could be represented by a simplified form of Eq. (1) :

$$
\frac{\partial C}{\partial t} = D_L \frac{\partial^2 C}{\partial x^2} - \bar{u} \frac{\partial C}{\partial x}
$$
 (2)

where

$$
D_{\underline{L}} = \text{longitudinal dispersion coefficient},
$$

\n
$$
\overline{u} = Q/A,
$$

\n
$$
Q = \text{flow rate, and}
$$

\n
$$
A = \text{cross-sectional area.}
$$

Thus, for a one-dimensional channel with a uniform cross-section and mean velocity, an exact solution to Eq. (2) for a point source and a fixed coordinate system is:

$$
C(x,t) = \frac{M}{A\sqrt{4\pi D_L t}} e^{-\frac{(x-\bar{u}t)^2}{4 D_L t}}
$$
 (3)

where

 $M =$ mass of the constituent introduced, and $x =$ distance downstream from the point of release.

Shih and Gloyna (1967) developed a transport equation for a one-*4 (* dimensional channel to predict dispersion as well as uptake and release from the sorption phases, In the general case, it has the form

$$
\frac{\partial C}{\partial t} = D_{L} \frac{\partial^{2} C}{\partial x^{2}} - \bar{u} \frac{\partial C}{\partial x} + \sum_{j=1}^{m} S_{j}
$$
 (4)

where

j *=* the index number for each sorption phase, and S_{1} $=$ uptake or release from the jth of m sorption phases.

Solutions to Eq. (4) are obtainable; however, difficulties arise in describing the dispersion coefficient and the sorption terms for the radionuclides., Therefore, considerable thought must be given to selecting dispersion coefficients and defining the various sources and sinks that are involved,

Longitudinal Mixing

Taylor (1954) was able to derive ^apredictive equation for the dispersion Taylor (1954) was able to derive a probability of the straight pipes, as

$$
D_{\mathbf{L}} = 10.1 \, \mathbf{r}_0 \, \mathbf{u}^* \tag{5}
$$

where

Some investigators have attempted to apply Taylor's expression to stream flow, Such applications are approximate, since there is no relation between the geometry or velocity distributions in stream flow and those occurring in a pipe.

Elder (1959) assumed that only the vertical velocity gradient is important in stream flow, and developed an expression analogous to Taylor's but with a coefficient equal to 5 .93,

$$
D_{L} = 5.93 \text{ Hu} \star \tag{6}
$$

where

H *.* ⁼depth of water.

Other investigators derived similar expressions for D_r and found that it is extremely sensitive to lateral velocity profiles. However, Elder's
expression seems to be quite adequate in one-dimensional situations where the channel is not too wide. For very wide channels, Fischer (1964) has shown that half—width,rather than depth,is the dominant scale and therefore is

important in defining the longitudinal dispersion coefficient, Such relations for the dispersion coefficient usually can be written in terms of the Manning Equation and other variables characteristic of stream channels*.*

Shih and Gloyna (1967), based on the results of their dye studies, were able to develop a relationship between the dispersion coefficient, $D_{L'}$, and channel velocity, \bar{u} . It was of the form:

$$
D_{L} = 29 \text{ (a)}^{0.9} \tag{7}
$$

where D_{τ_L} had units of 10^{-2} ft²/sec and \bar{u} had units of 10^{-3} ft/sec. Armstrong and Gloyna (1968) found that using this equation for the dispersion coefficient in their model overpredicted the cloud dispersion and underestimated its velocity. This same observation was verified in the course of this study.

Armstrong and Gloyna (1968) also used observed concentration curves from their study to obtain dispersion coefficients for the model river. These data are shown in Fig. 1. All the dispersion coefficients, D_r, obtained from the flume studies under various flow conditions, were fitted to a generalized equation in the form:

$$
D_{\underline{L}} = 3.26 \text{ (}\bar{u}\text{)}^{0.607} \tag{8}
$$

where D_{L} had units of ft^2/min and \bar{u} had units of ft/min . This equation gives dispersion coefficients which seem to work very well for the model river, However, one should not try to extrapolate this equation to other systems a s it holds true for the flume only and even then only under a small range of conditions *.*

Sources and Sinks

In general, the sorption terms for plants and bottom sediments have the following form:

$$
S_j = K_j [W_j - g_j (C)] \tag{9}
$$

where

$$
K_j =
$$
 the mass transfer coefficient for phase j ,
\n $g_j(C) =$ the transfer function relating the concentration of activity
\nin water to the equilibrium level in phase j , and

 W_i = the specific activity in the jth of m sorption phases.

The activity in W_j is determined by:

$$
\frac{\partial W}{\partial t} = K_j [g_j(C) - W_j]
$$
 (10)

Usually the equilibrium concentration of radionuclide in a sorbent, g(C) , has the Freundlich isotherm form,

$$
g(C) = KCn
$$
 (11)

where K and n are constants pertaining to a given radionuclide and sorption phase. For uptake of most radionuclides $n = 1.0$ and K becomes Kd, the equilibrium distribution coefficient. Thus, the,non—equilibrium radionuclide sorption reaction within a given material is derived as ,

$$
\frac{\partial W}{\partial t} = K_j [Kd_j C - W_j]
$$
 (12)

and it follows that,

$$
S_j = K_j [W_j - K d_j C]
$$
 (13)

MODEL DEVELOPMENT

Equation Development

Since the dispersion equation is written as a function of time, T , and distance, L , let i and n be increments of the variables x and t where $x = L/I$, I being an integer, and $t = T/N$, N being an integer. The set of points in the x-t plane forms a net and is given by $x = i \Delta x$ and of points in the x-t plane forms a net and is given by $x = i\Delta x$ and
t = $n\Delta t$, where i = 1, 2, ..., I and n = 0, 1, 2, ..., N. The concen $t = n\Delta t$, where $i = 1, 2, ..., I$ and $n = 0, 1, 2, ..., N$. The concentration, C, at each mesh point is approximated by C($i\Delta x$, $n\Delta t$) which is tration, C, at each mesh point is approximated by C(i Δx , n Δt) which is
denoted by C_iⁿ. Using the implicit method in which derivatives are approximated by expanding $C_i^{\{1\}}$ in a Taylor series and averaging over the time step, Δ t, the dispersion equation may be written as:

$$
\frac{C_{i}^{n+1} - C_{i}^{n}}{\Delta t} = \frac{D_{L}}{2} \left\{ \frac{(C_{i+1}^{n+1} - 2C_{i}^{n+1} + C_{i-1}^{n+1})}{\Delta x^{2}} + \frac{(C_{i+1}^{n} - 2C_{i}^{n} + C_{i-1}^{n})}{\Delta x^{2}} \right\}
$$
\n
$$
-\frac{\pi}{2} \left\{ \frac{(C_{i+1}^{n+1} - C_{i-1}^{n+1})}{2 \Delta x} + \frac{(C_{i+1}^{n} - C_{i-1}^{n})}{2 \Delta x} \right\} \tag{14}
$$

where

1 *=* **1,2,** *a* ,, l, and $n = 0, 1, 2, \ldots, N$.

The rigor for this method has been established by Smith (1965). The boundary conditions for instantaneous release are

$$
C_i^0 = 0; i = 1, 2, ..., I
$$

\n
$$
C_i^n = 0 \text{ as } i \to \infty
$$

\n
$$
C_i^n = \text{finite value as } n \to \infty
$$

and the initial condition is:

$$
C_{\circ}^{t+t_{\circ}} = \frac{M}{A\sqrt{4\pi D_{L}(t+t_{\circ})}} = \frac{\left[\bar{u}(t+t_{\circ})\right]^{2}}{e}
$$
\n(15)

where

= a time slightly greater than zero for which a finite solution t_{\circ} for Eq. (15) can be obtained.

For a continuous release, the boundary condition is:

$$
C_O^{\mathbf{n}} = \frac{M}{QT}
$$
 (16)

for all n where T is the time span over which the continuous release occurs.

Eq. (14) may also be expressed as:

$$
a C_{i-1}^{n+1} + b C_i^{n+1} + c C_{i+1}^{n+1} = \frac{D_L \Delta t}{2 \Delta x^2} \left(C_{i+1}^n - 2 C_i^n + C_{i-1}^n \right)
$$

$$
- \frac{\bar{u} \Delta t}{4 \Delta x} \left(C_{i+1}^n - C_{i-1}^n \right) + C_i^n
$$

$$
a = - \frac{D_L \Delta t}{2 \Delta x} \frac{\bar{u} \Delta t}{2 \Delta x} \tag{17}
$$

where

 \sim .

$$
=\frac{L}{2\Delta x^2} - \frac{d\Delta t}{4\Delta x} \tag{18}
$$

$$
b = 1 + \frac{D_{L} \Delta t}{\Delta x^{2}}
$$
, and (19)

$$
c = -\frac{D_L \Delta t}{2 \Delta x^2} + \frac{\overline{u} \Delta t}{4 \Delta x} \qquad (20)
$$

For the transport equation with sorption terms, Eq. (17) becomes:

$$
\mathsf{a}\, \mathsf{C}_{i-1}^{n+1} + \mathsf{b}\, \mathsf{C}_i^{n+1} + \mathsf{c}\, \mathsf{C}_{i+1}^{n+1} \ = \ \frac{\mathsf{D}_L\, \Delta\, \mathsf{t}}{2\, \Delta\, \mathsf{x}^2} \left(\mathsf{C}_{i+1}^n - 2\, \mathsf{C}_i^n + \mathsf{C}_{i-1}^n\right)
$$

$$
-\frac{\overline{u}\Delta t}{4\Delta x}\left(C_{i+1}^{n}-C_{i-1}^{n}\right)+\Delta t\sum_{i=1}^{m}K_{j}\left[W_{j,i}^{n}-Kd_{j}C_{i}^{n}\right]
$$
\n(21)

Bottom Sediments - For bottom sediments Shih and Gloyna (1967) used Eq. (12) in the following form:

$$
\frac{\partial W_{1,i}}{\partial t} = K_1 [Kd_1 C_i - W_{1,i}]
$$
 (22)

and Eq. (13) as:

$$
S_{1,i} = \frac{K_1}{HA_S} [W_{1,i} - Kd_1C_i]
$$
 (23)

where

 $A_{\rm S}$ *⁼*cross-sectiona1 area of ^asediment sample, and ^H**=** effective depth of sediments.

In finite-difference form Eq. (22) and Eq. (23) become:

$$
W_{1,i}^{n} = W_{1,i}^{n-1} + \Delta t K_{1} [K d_{1} C_{i}^{n-1} - W_{1,i}^{n-1}]
$$
 (24)

and

$$
S_{1,i} = \frac{K_1}{HA_s} \left[W_{1,i}^n - K d_1 C_i^n \right] . \tag{25}
$$

Plants - For plants Armstrong and Gloyna (1968) in a similar fashion used Eq. (12) and Eq. (13) in finite difference form as:

$$
W_{2,i}^{n} = W_{2,i}^{n-1} + \Delta t K_2 [Kd_2 C_i^{n-1} - W_{2,i}^{n-1}]
$$
 (26)

and

$$
S_{2,i}^n = Mb K_2 \left[W_{2,i}^n - K d_2 C_i^n \right]
$$
 (27)

where

= biomass of plants. Mb

With the sorption terms for bottom sediments and plants included, Eq. (21) becomes:

$$
a C_{i-1}^{n+1} + b C_i^{n+1} + c C_{i+1}^{n+1} = \frac{D_L \Delta t}{2 \Delta x^2} \left(C_{i+1}^n - 2 C_i^n + C_{i-1}^n \right)
$$

$$
- \frac{\overline{u} \Delta t}{4 \Delta x} \left(C_{i+1}^n - C_{i-1}^n \right) + \frac{K_1 \Delta t}{H A_s} \left(W_{1,i}^n - K d_1 C_i^n \right)
$$

$$
+ M b \Delta t K_2 \left(W_{2,i}^n - K d_2 C_i^n \right) \tag{28}
$$

where

 $= 1, 2, ..., I$ and $\rm i$ $= 0, 1, ..., N.$ n

Solution Technique

If Eq. (28) is rewritten at some point in time, n, for all values of i in matrix notation it becomes $AC = d$ or

- $\rm C$ $=$ represents the column matrix of unknowns, and
- $\mathbf d$ $=$ represents the column matrix of known quantities in Eq. (28).

The matrix [A] is tridiagonal since any row excluding the top and bottom rows contains only three terms, the diagonal and two immediately adjoining off diagonal terms *.* The bottom and top rows which express the boundary conditions contain the diagonal and one offdiagonal term *.*

. Eq. (29) may be solved by a number of different methods. The solution methods differ considerably in computational effort and hence in computer cost. For the problem at hand a unique and highly efficient solution method described by Ralston and Wilf (1967) was used.

Briefly, this algorithm takes advantage of the fact that the matrix $[A]$ is tridiagonal, hence the algorithm is very simple and fast. The algorithm is recursive, allowing the following sequence of steps:

- (1) Set $f_1 = c_1/b_1$ and $g_1 = d_1/b_1$
- (2) Then operate from row 2 to the last row, I, using the Then operate from row 2 to the last row, I, using the
recursive relations below for i = 2, I. Compute

$$
f_i = \frac{c_i}{b_i - a_i f_{i-1}}
$$

$$
g_{i} = \frac{d_{i} - a_{i}g_{i-1}}{b_{i} - a_{i}f_{i-1}}
$$

Store these quantities since

$$
C_i^{n+1} = g_i - f_i C_{i+1}^{n+1}
$$
 (30)

The last row, I, is such that

$$
C_{I}^{n+1} = g_{i}
$$

(3) With C_r^{n+1} computed, operate with Eq. (30) from row I-1 to row 1, i.e., back substitution.

The back substitution yields the set of concentrations , $\text{C}^{\text{n+1}}$, to advance the solution over the time step Δt .

 λ

 $\label{eq:1} \mathbf{x}_\alpha \mathbf{x}_\alpha \mathbf{x}_\beta + \mathbf{y}_\alpha \mathbf{x}_\beta \mathbf{x}_\beta + \mathbf{y}_\alpha \mathbf{x}_\beta$

DISCUSSION

In compliance with the objective of this study, a mathematical model has been developed in a form suitable for simulation on a digital computer for routing a radionuclide through a model river system (flume) .

Model Capability

The model was designed so that it has the following capabilities and characteristics:

- (1) It distributes radionuclide activity by advective and dispersional mechanisms along the longitudinal axis of the system.
- (2) It may be discretized intoany number of segments (vertical planes normal to the longitudinal axis) as may be appropriate to describe spatial variations in radionuclide activity.
- (3) Itis capable of treating instantaneous, continuous, or time varying releases of radionuclide activity.
- (4) It provides for a temporal description of radionuclide activity throughout the system.
- (5) It provides for sorption and desorption by both plants and bottom sediments.

Verification, Application, and Results

The results obtained from the dye-release data, Appendix A, are illustrated in Figs. 2a and 2b. The shapes of the dye curves at the four stations on the east side of the flume, Fig. 2a, were well predicted except for the peaks. From the shape and maximum values of the observed data, it is
apparent, as Fischer (1966b) has pointed out, that initial dispersion of a point source does not follow Taylor's Eq. (2), but rather takes the shape of ^a skewed normal distribution because of the dominance of convection over diffusion. However, at some point downstream, the curves approach a form where the Taylor expression is valid. The point is made, however, that dispersion was well predicted and velocity was only slightly overestimated. The

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FIG. 2a. OBSERVED AND PREDICTED DYE STUDY CURVES

FIG.2b. OBSERVED AND PREDICTED DYE STUDY CURVES

results of the west side, Fig. 2b, again show that dispersion and velocity were fairly well predicted except for the 90—ft. station.

The results of this part of the study verified the observation of Armstrong and Gloyna (1968). When they applied Eq. (7) used by Shih and Gloyna (1967) their predicted curve overestimated the cloud dispersion and underestimated the velocity; however, when they used dispersion coefficients determined from their own studies,very good agreement between observed and predicted curves was obtained.

The results obtained with a sorption term for bottom sediments added to the dispersion equation were predicted using the factors in Appendix *A* and are shown in Fig. 3 *.* The fit to the observed data was good, although,as in the dye studies, velocity was slightly overestimated. Again, when Eq. (7) was used to determine the dispersion coefficients, the predicted curves overestimated the cloud dispersion; however, when Eq. (8) , developed in this study, was used, good agreement was obtained under test conditions **.**

The results obtained with ^asorption term for plants added to the dispersion equation are shown in Fig. 4. The agreement between the predicted and observed curves was extremely good in this instance.

Continuous releases of radionuclides may also be modeled with this numerical solution. Using data taken by Armstrong and Gloyna (1968),
an equilibrium level of 53 dpm/ml was inserted into the model and the curve illustrated in"Fig. 5 was obtained. The transport equation with sorption terms for both bottom sediments and plants was used in the continuous release.

Application to a Real River

In light of the results obtained in this study, the utility of this model has been sufficiently demonstrated; however, it should be recognized that the model does have its limitations*.* Thus it seems appropriate at this point to consider how the model might be adapted to a real river system.

Model Resolution and Sensitivity - The mode of conceptually representing a natural conveyance channel will depend to a considerable degree on the detail required in the space and time description of the radio nuclide activity. If flows are steady and the geometric properties rather

FIG.3. INSTANTANEOUS RELEASE CURVES FOR WATER AND SEDIMENTS

FIG.4. INSTANTANEOUS RELEASE CURVES FOR WATER AND PLANTS

FIG.5. CONTINUOUS RELEASE CURVES FOR WATER AND PLANTS

uniform from place to place, as for example in the flume, it is sufficient to represent the system with a few prismatic segments of fixed geometry. The length of channel segment depends, in such cases, more on the variations in-input data than on flow or cross-section configuration, the optimum length being chosen to provide the necessary detail required to describe the radionuclide activity along the axis of flow. - **I**

However, if the flows are nonsteady, with large changes from time to time in discharge, water depth, water surface area, and velocity, it may be necessary to discretize the system into a greater number of elements *.* The choice of number and size of individual elements may be dictated, in part, by the technique by which nonsteady flows are determined.

Transport —In natural channels wide variation in geometry may be expected along the axis of flow and the effects of these on dispersion and convective transport may be further magnified by the inherent unsteadiness of natural flows *.* Consequently, in such cases, a satisfactory description of the radionuclide transport will probably require maximum detail. This might entail a need to look at two-dimensional modeling, i.e., lateral
dispersion and convection as well as longitudinal.

Sources and Sinks - Although hydrodynamic mixing is believed to be the dominant factor involved, it is recognized that the interaction of radionuclides associated with the liquid phase and various solid phases, i.e., the biota, the bottom sediments, and the suspended debris, etc., of a river may pro'duce a significant effect on the net transport of radionuclides. These components or sorption phases manifest themselves in time—concentration relationships as previously described. The mass-transport and distribution coefficients used in these relationships vary with contact time, temperature, velocity, type of sediment, etc. Thus, to be able to adequately describe the effects of these various components a detailed knowledge of the biota, types of sediments , and sediment transport characteristics of a natural river will be required.

Data Reguirements **—**The following brief discussion presents the data requirements for what may be regarded as a normal river simulation problem.

(l) Hydraulic Data

- (a) For steady flow: water surface area of each channel segment. For unsteady flow: depth—surface area curve for each channel segment.
- (b) For steady flow: length and cross—sectional area of each channel segment.
	- For unsteady flow: length and depth—cross-sectional area curve for each channel segment.
- (c) Longitudinal dispersion: velocity profiles, roughness, and sinuosity of stream.
- (d) Waste discharge: amount, quality, and location.
- (e) Tributary inflows: amount, quality, and location.
- (2) Radionuclide Data
	- (a) Detailed description of release conditions and amount released.
	- (b) Spatial and temporal description of radionuclide activity after release. This will require a comprehensive sampling program throughout the river system. This data can be used to compute dispersion coefficients which in turn can be used to check against dispersion coefficients computed empirically from the hydraulics and geometry.
- (3) Environmental Data
	- (a) Detailed description of the biota throughout the river system.
	- (b) Detailed description of the bottom sediments throughout the river system.
	- (c) Detailed description of the sediment transport characteristics throughout the river system.

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APPENDICES

APPENDIX A - DATA — RADIONUCLIDE TRANSPORT MODEL

1. Dye Release Data (after Armstrong **-** 1968)

a. East Side

^M*=* 1000 ^m ^g $Q = 5.15 \text{ cfm}$ $A = 1.56$ ft² $D_r = 8.0 \text{ ft}^2/\text{min}$ b. West Side ^M*=* 1000 ^m ^g Q *=* 5.15 cfm $A = 1.56$ ft² $D_L = 6.0 \text{ ft}^2/\text{min}$

2. Instantaneous Release Data for Sediments (after Shih - 1967)

 $M = 0.55 \,\mu c$ Q *=* 1.93 Cfm $A = 1.04 \text{ ft}^2/\text{min}$ D_{L} = 2.6 ft²/min $a^2 = 4.16 \times 10^{-3}$ ft² k_1 = 1.83 x 10⁻⁴ min⁻¹ Kd_1 = 140 dpm/core/dpm/ml

3 . Instantaneous Release Data for Plants (after Armstrong *-* 1968)

M = 0.504 \n
$$
\mu
$$
C
\nQ = 1.67 \n cfm
\nA = 1.04 \n ft^2
\nD_L = 2.30 \n ft^2/min
\nMb = 9.04 \n \times 10⁻⁵ \n gm/ml
\n k_2 = 5.0 \n \times 10⁻⁴ \n min^{-1}
\n Kd_2 = 260 \n dpm/gm/dpm/ml

4. Continuous Release Data for Plants (after Armstrong. *—*1968) ^M*=* 2 .08 ⁿ ^o

M = 2.08 \n
$$
\mu
$$

\nQ = 0.54 cm
\nA = 1.04 ft²
\nD_L = 1.0 ft²/min
\nMb = 9.04 x 10⁻⁵ gm/ml
\n k_2 = 5.0 x 10⁻⁴min⁻¹
\nKd₂ = 260 dpm/gm/dpm/ml

APPENDIX B *-* COMPUTER PROGRAM *-* RADIONUCLIDE TRANSPORT MODEL

Data Input

^Arelatively small amount of data is required for use of the program. The data may be grouped as follows:

- 1. Title of study
- Control **2**
- *.* Time and space dimensions 3
- Initial conditions and hydraulics 4
- 5 *.* Parameters and coefficients for bottom sediments
- Parameters and coefficients for plants 6
- 7. Printout control
- . Printout titles

The quantity identification, corresponsing units, and related format specifications are given as:

 $\label{eq:1} \theta$

 ϵ

RESTRICTIONS

- l. The maximum number of elements or reaches is fixed at 500*.*
2. No more than 500 printout times are allowed.
- 2. No more than 500 printout times are allowed.
3. No more than 6 locations can be printed out.
-
- 4. The only restriction on the total time for which the program is allowed to run is that TMAX/DELT *S* 500.
- is allowed to run is that $\text{TMAX}/\text{DELT} \leq 500$.

5. The program is economical to employ. As an example
 $\frac{180 \text{ min of real time can be simulated on the INNVAC}}{180 \text{ min of real time.}}$ The program is economical to employ. As an example
180 min of real time can be simulated on the UNIVAC
1108 system in approximately 15 ses (less than 5 ses 1108 system in approximately 15 sec (less than 5 sec on CDC 6600 System).

PROGRAM LISTING

A listing of the program is presented on the following pages.

PROGRAM LISTING

 C * C C THIS PROGRAM IS AN IMPLICIT-FINITE-DIFFERENCE MODEL Ć C WHICH WILL ROUTE A RADIONUCLIDE THROUGH A MODEL C C RIVER SYSTEM (FLUME). IT PROVIDES FOR --C C 1. TRANSPORT BY DISPERSION AND ADVECTION \subset C 2. SORPTION AND DESORPTION BY BED SEDIMENTS ζ ϵ 3. SORPTION AND DESORPTION BY PLANTS C ϵ 4. INSTANTANEOUS RELEASES \overline{C} ϵ 5. CONTINUOUS RELEASES \subset * * * * * * * * * * * * * $\sqrt{2}$ \mathcal{H} ϵ DIMENSION CONC(500), CONCN(500), IFLAG(500), A(500), B(500), C(500), ¥ $D(500)$, CBS(500), CBSN(500), CP(500), CPN(500), IPR(6), ¥ $CPR1(500,6)$, TITLE(6), Z(500), TIM(500) REAL LENGTH, KS, K1, KP, K2, MCTDPM $PI = 3.1416$ * * * * * * * * * * * * * * * ϵ \subset \mathcal{C} MCTDPM CONVERTS MICROCURIES TO DPM C \mathcal{C} FITOCM CONVERTS FEET TO CENTIMETERS \subset ϵ CFTTML CONVERTS 1/FT**3 TO 1/ML C * * * * * * * * * * * * * * * * ϵ $MCTDPM=2.22E+09$ $FTTOCM=30.45$ $CFTTML=3.54E-05$ < * * * * * * * * * * * * * * * * * * C C STEP 1 -- READ NAME OF RADIONUCLIDE C **C * * * * * * * * * * * * * * * * *** ₩ \subset READ 1, RADNUC 1 FORMAT (12A6) \subset C 2 -- READ TYPE OF RELEASE AND PRINT CONTROL C STEP C C MODE = 1 FOR INSTANTANEOUS RELEASE \subset $\mathsf C$ \subset MODE = 2 FOR CONTINUOUS RELEASE C NPR = NO. OF LOCATIONS TO BE PRINTED OUT \subset * * * * * * * * * * * * * * * -34 \mathbf{R} C READ 2, MODE, NPR 2 FORMAT (215) \subset C ϵ STEP 3 -- READ TIME AND SPACE DIMENSIONS C \subset \subset DELT = TIME INTERVAL (MIN) ζ ϵ TMAX = LENGTH OF TIME AXIS (MIN) $\mathsf C$ C $DELX = SPACE INTERVAL$ (FT) C LENGTH = LENGTH OF SPACE AXIS (FT) C

 ϵ $*$ \subset READ 3, DELT, TMAX, DELX, LENGTH 3 FORMAT (8F10.0) \subset * * * * C C STEP \overline{u} -- READ INITIAL ACTIVITY AND HYDRAULIC CONDITIONS C CBKGRN = BACKGROUND ACTIVITY (DPM/ML) Ċ C \subset COMASS = TOTAL ACTIVITY RELEASED (MICROCURIES) Ċ C $QFLOW = INFLOW RATE OF WATER (CFM)$ Ć C AREA = X-SECTIONAL AREA (FT**2) C C DEPTH = WATER DEPTH (FT) C $\mathcal{C}_{\mathcal{C}}$ DL = LONGITUDINAL DISPERSION COEFFICIENT (FT**2/MIN) C * * * * * (READ 3, CBKGRN, COMASS, GFLOW, AREA, DEPTH, DL * * * * * * * * * * * $\sqrt{2}$ C 5 -- READ COEFFICIENTS FOR BED SEDIMENTS C STEP \subset ζ \mathcal{C} $K1$ = MASS TRANSFER COEF. (1/MIN) C \subset $KS = FQUILIBRIUM DISTRIBUTION COEF. (ML/CORE)$ C $AB = SAMPLING AREA OF SEDIMENTS IN CORE (FT**2)$ C $*$ \subset C -¥⊦ 圣 ¥. $RFAD 3, K1, K5, AR$ \subset * * * * * * * * * * * * * \subset 6 -- READ COEFFICIENTS FOR PLANTS $\mathsf C$ STEP \subset \subset \subset $K2 = MASS$ TRANSFFR COFF. (1/MIN) C \subset $KP = EQUILIBRIUM DISTRIBUTION COFF. (ML/GM)$ C \subset BIOMSS = BIOMASS OF PLANTS $(GMS/ML**3)$ * * * * * * * * * * * * * * * * * * * \subset $\mathcal{C}_{\mathcal{C}}$ 兴 $\boldsymbol{\mathcal{X}}$ READ 3, K2, KP, BIOMSS * * * * * \subset \subset 7 -- READ INDEXES OF LOCATIONS TO BE PRINTED OUT STEP \subset READ $4, (1PP(1), I=1,NPR)$ 4 FORMAT (615) * * * * * * C STEP -- READ DISTANCES FROM SOURCE FOR POINTS TO BE PRINTED OUT C C 8 C TITLE = $(XX-FT)$ \subset * * * * * * * * * C -¥∹ ∗ READ 1, (TITLE(I), $I=1$, NPR) PRINT 2055 2055 FORMAT (1H1) \subset * -* * * * * * * * * * * * ⋇ ∗ ⋇ C 9 -- ECHO PRINT ALL INPUT STEP DATA C \ast ÷.

```
PRINT 11, RADNUC
   11 FORMAT (10X, 15HINPUT DATA FOR, A6, 6H STUDY, //)
      PRINT 12, PTIME, NPR
   12 FORMAT (15X, F10.2, I5, /)
      PRINT 13, DELT, TMAX, DELX, LENGTH
   13 FORMAT (15X, 4F10, 2, 7)PRINT 14, CBKGRN, COMASS, QFLOW, AREA, DEPTH, DL
   14 FORMAT (15X, 8F10.3, /)
      PRINT 15, K1, KS, AR
   15 FORMAT (15X,F10.6,F10.2,F10.5,/)
      PRINT 16, K2, KP, BIOMSS
   16 FORMAT (15X, F10.6, F10.2, F10.7, 7)
      PRINT 17, (IPR(I), I=1, NPR)
   17 FORMAT (15X, 1615, /)
      PRINT 18, (TITLE(I), I=1, NPR)
   18 FORMAT (15X, 12A6, /)
      VEL=QFLOW/AREA
      V04DX=VEL/(4.0*DELX)DONX2 = DL / (2.0 * DELX * DELX)COMASS=COMASS*MCTDPM*CFTTML
      PTIMF=DELT
      DEPTH=DEPTH*FTTOCM
      AP = AP * (FTTOCM) * * 2NMAX=LENGTH/DELX+1
      NMAXL1 = NMAX-1IF (MODE.EQ.1) GO TO 88
      TIME = 0.0CSTART=COMASS/TMAX/QFLOW
      GO TO 87
   88 DELT=DELT/8192.0
      TIME=DFLT
      CSTART=C.5*COMASS/(AREA*SQRT(PI*DL*DELT))*FXP(-(VEL*DELT)**2/
             (4.0*PL*DFLT)87 CONTINUE
\subset\zetaSTEP 10 -- SET FLAG FIELD TO FIX BOUNDARY CONDITIONS FOR EACH REACH C
\mathsf CIFLAG = 1 FOR EXT. BOUNDARY CELL (INST. RELEASE PT)
                                                                         C
\epsilonIFLAG = 2 FOR INT, BOUNDARY CELL ADJ, TO RELEASE
                                                                         \mathsf{C}\subsetIFLAG = 3 FOR INT. CELL NOT ADJ. TO A BOUNDARY
                                                                         \subset\subsetIFLAG = 4 FOR INT. BOUNDAPY CELL FOR
                                                          \mathcal{C}X = 0\mathcal{C}C/\epsilonIFLAG = 5 FOR EXT. BOUNDARY CELL FOR
                                                               x = 0\mathsf{C}IFLAG = 6 FOR EXT. BOUNDARY CELL (CONT. RELEASE PT)
\subset\subsetDO 5 I = 1.5NMAXCONCN(1)=CBKGRNIF (I \cdot NE \cdot 1) GO TO 6
      IFLAG(I)=1IF (MODE, NE, 1) IFLAG(I)=5
      CONC(I) = CSTARTGO TO 5
    6 IF (I.NE.2) GO TO 7
      IFLAG(I)=2CONCH) = CBKGRN
```

```
CRS(1) = CBKGRNCP (I) = CBKGRN
     GO TO 5
   7 IF (I.NE.NMAXL1) GO TO 8
     IFLAG(L) = 4CONC(1) = CBKGRNCBS(I) = CBKGRNCP(1) = CBKGRNGO TO 5
   8 IF (I.NE.NMAX) GO TO 9
     IFLAG(I) = 5CONC(I)=CBKGRN
     G0, T0.59 IFLAG(I)=3
     CONCUI) = CBKGRNCPS(I) = CBKGRNCP(1) = CBKGRN5 CONTINUE
     NTT=-1M = 1TIM(M) = TIMMETMAX=TMAX-0.1PTIME=PTIME-0.1
     DO 2O I = 1. NPRK = I PR (I)\sim 10CPR1(M, I) = CONC(K)20 CONTINUE
     PRINT 2055
     PRINT 2054, RADNUC
 2054 FORMAT (39X,9HCOMPUTED, A6,15H CONC. (DPM/ML), //,53X,2HVS,//,
             44X, 20HDISTANCE FROM SOURCE, //)
    *PRINT 2C56, (TITLE(I), I=1, NPR)
 2056 FORMAT (19X,4HTIME,6X,6(4X,A6))
     PRINT 165, TIME, (CPR1(M, I), I=1, NPR)
C STEP 11 -- COMPUTE COEFFICIENT AND VECTOR MATRICES
                                                                    \subset\Delta t\star\mathbf{x}\epsilon09 TIME=TIME+DELT
     VTO2DX=DELT*VO4DX
     DO2DX2 = DELT * DODX2DO 100 I=1.9 NMAX
     IFL = IFLAG(I)GO TO (101,102,103,104,105,100), IFL
  101 CONCN(I)=0.5*COMASS/(AREA*SQRT(PI*DL*TIME))*EXP(-(VEL*TIME)**2/
              (4.0*DL*TIME)GO TO 100
  105 CONCN(I)=CSTART
     GO TO 100102 ITPID=IA(1) = -(VTO2DX+DO2DX2)B(1) = 1.0 + 2.0 * D02DX2C(1) = VTO2DX-DO2DX2SOBS=K1/I (DEPTH*AR)*(CBS(I)-KS*CONC(I))
```

```
CBSN(I)=CBS(I)+DFLT*K1*(KS*CONC(I)-CBS(I))
     SOP = BIONSS*K2*(CP(1)-KP*CONCL))CPN(1)=CP(1)+DELT*K2*(KP*CONC(1)-CP(1))D(I) = DO2DX2*(CONC(I-1)-2*0*CONC(I)+CONC(I+1))+VTO2DX*(CONC(I+1)-CONC(I-1))-A(I)*CONCN(I-1)+CONC(I)+*
         (SOBS+SOP)*DFLT
    G0 TO 100103 A(1) = -(VTO2DX+DO2DX2)B(I) = 1.0 + 2.0 * DO2DX2C(1) = VTO2DX - DO2DX2SORS=K1/IDEPTH*AR)*(CBS/I)-KSSCONC(I))CBSN(I) = CBS(I) + DFLT*K1*(KS*CONC(I) - CBS(I))SOP=BIOMSS*K2*(CP(I)-KP*CONC(I))
     CPN(I) = CP(I) + DELT*K2*(KP*CONCI) - CP(I))D(I) = DO2DX2*(CONC(I-1)-2*C*CINC(I)+CONC(I+1))-VTO2DX*(CONCI+1)-CONCI-I-1)+CONCI+RSOES+SOP) * DELT
    ₩.
    GO TO 100
 104 NTRID=I
     A(I) = -(VTO2DX+DO2DX2)P(I) = 1.0 + 0.2 X2 + VTO2 DXC(1) = VTO2DX - NO2DX2SORS=K1/(DFPTH*AR)*(CBS(1)-KS*CONC(1))CBSN(I) = CBS(I) + DELT*K1*K(S*CONC(I) - CBS(I))SOP = BIONSS*K2*(CP(I)-KP*CONCI))CPN(1)=CP(1)+DELT*K2*(KP*CONC(1)-CP(1))D(I) = DO2DX2*(CONC(I-1)-2=0*(-ONC(I)+(CONC(I+1))-VTO2DX*(CONC(I+1)-CONC(I-1))+CONC(I)+(SOBS+SOP)*DELT
    *
 100 CONTINUE
* * *
                                                              \epsilonC STEP 12 -- SOLVE TRIDIAGONAL MATRIX
\mathcal{N}CALL TRIDAG(Z,A,B,C,D,ITRID,NTRID)
     DO 110 I=ITRID, NTRID
     CONCN(I)=Z(I)110 CONTINUE
     CONCN(NMAX) = CONCN(NMAXL1)STEP 13 == REPLACE OLD SOLUTIONS WITH NEW SOLUTIONS AT TIME + DELT
                                                             \epsilonDO 130 I=1.9 NMAX
     CONCH = CONCN(I)
     CPS(I) = CBSN(I)CP(1)=CPN(1)130 CONTINUE
     IF (TIME.GT.PTIME) GO TO 95
     DFLT = 2.0*DFLT50T12595 DELT=PTIME+0.1
     M = M + 1TIM(M)=TIMF
```
* * * * $*$ \subset ϵ $*$ ∗ C STEP 14 -- PRINT OUT SELECTED LOCATIONS IN SYSTEM $\mathsf C$ \overline{C} 兴 يد

 \sim

```
DO 150 I=1, NPR
    K = I PR (I)CPR1(M, I) = CONC(K)150 CONTINUE
    NTT = NTT + 1IF (NTT.NF.30) GO TO 164
    NTT = 0PRINT 2055
    PRINT 2054, RADNUC
    PRINT 2056, (TITLF(I), I=1, NPR)
164 CONTINUE
    PPINT 165, TIME, (CPR1(M, I), I=1, NPR)
165 FORMAT (18X, F5.1, 6X, 6F10.2)
125 CONTINUE
    IF (TIME.LT.TMAX) GO TO 99
    FND
```
SUBROUTINE TRIDAG (Z,A,B,C,D,ITRID,NTRID)

 $\sim 10^{-11}$

 $\boldsymbol{\theta}$

 $\sim 10^{-11}$

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 $\sim 10^{-11}$

 \mathcal{A}