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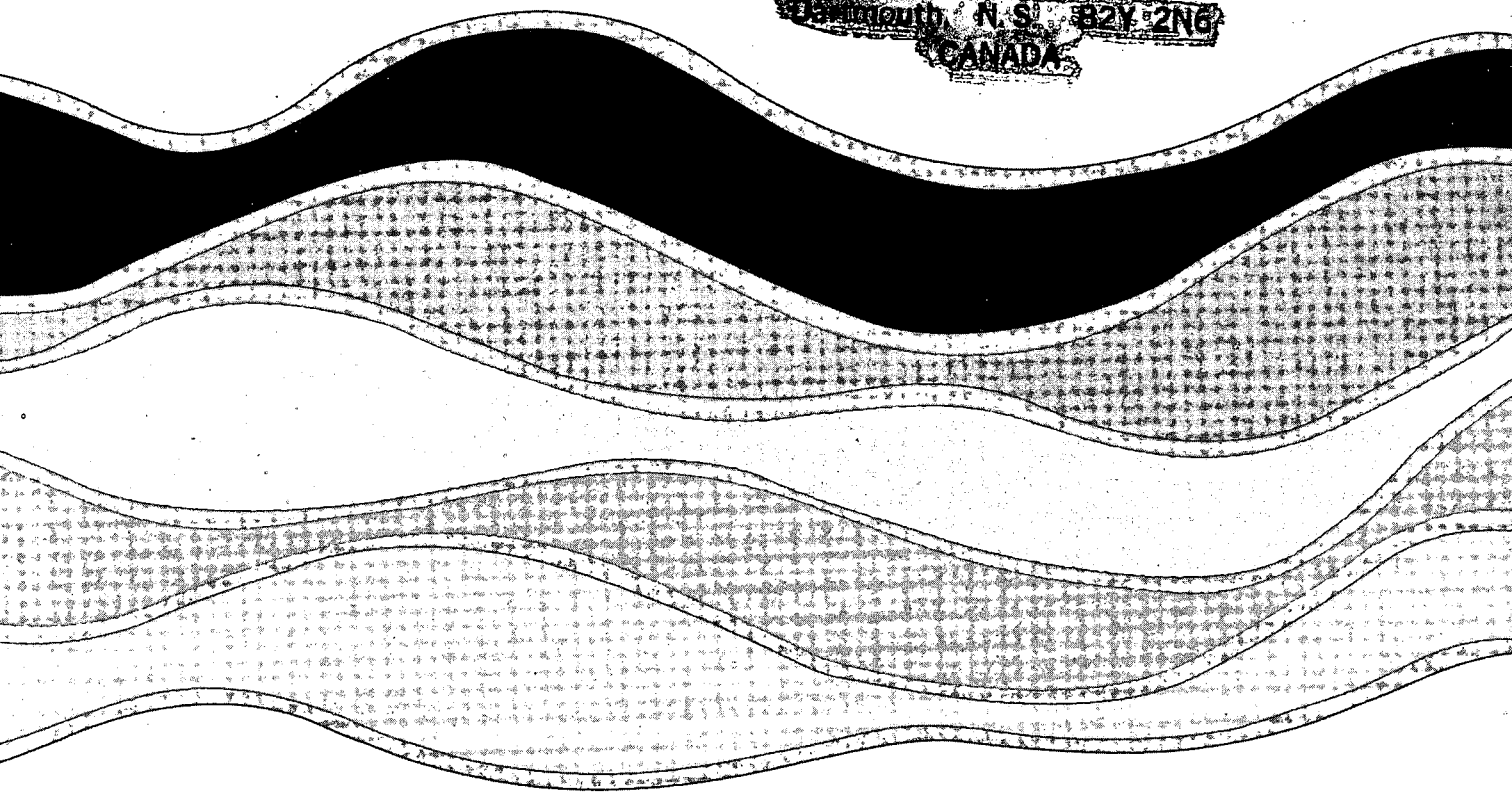

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NWRI CONTRIBUTION 90-87

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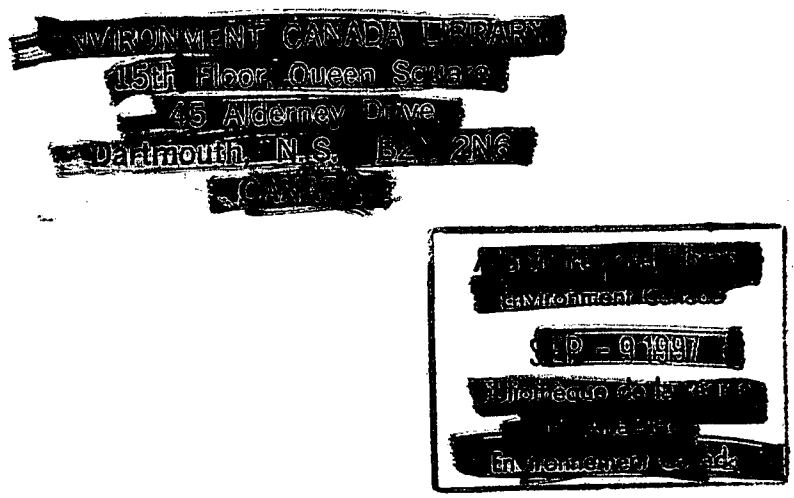

NUMERICAL SIMULATION OF CHEMICAL WASTE CONTAMINATION IN A SMALL STREAM

by

A.G. Bobba, D.C.L. Lam, W.G. Booty
and S.R. Joshi

Rivers Research Branch
National Water Research Institute
Canada Centre for Inland Waters
Burlington, Ontario L7R 4A6

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Management Perspective:

Many industrial and municipal waste discharges enter small streams rather than large rivers or lakes. In order to accurately determine the fate of these chemicals in such systems and to be able to design critical loads as part of the Canadian Environmental Protection Act or, in Ontario, as part of the MISA program; more sophisticated models need to be developed and applied. This presentation describes a model which incorporates a specialized function for the adsorption of organic and inorganic contaminants by bottom sediments and plants.

PERSPECTIVE ADMINISTRATIVE

De nombreux rejets industriels et municipaux sont évacués dans de petits cours d'eau plutôt que dans de grands cours d'eau ou des lacs. Pour être en mesure de déterminer avec justesse le devenir des déchets chimiques dans ces cours d'eau et d'établir les charges critiques dans le cadre de la Loi canadienne sur la protection de l'environnement ou, en Ontario, du programme MISA, il faut mettre au point et utiliser de meilleurs modèles. Le présent document décrit un modèle qui incorpore une fonction spécialisée prenant en compte les phénomènes d'adsorption des contaminants organiques et inorganiques par la végétation et les sédiments de fond.

Abstract:

A numerical model has been developed for routing chemical waste contamination through a small stream system. The capabilities of this simulation model include the following characteristics: a) It distributes contamination by advection and dispersion along the longitudinal axis of the system. b) 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 chemical contamination. c) It is capable of treating instantaneous, continuous, or time varying releases of chemical waste contamination. d) It provides for temporal description of contamination throughout the system. e) It provides for adsorption and desorption by both vegetation and bottom sediments.

RÉSUMÉ

On a mis au point un modèle numérique du devenir des déchets chimiques dans les petits cours d'eau. Ce modèle de simulation possède de nombreuses caractéristiques: a) il distribue la contamination par advection et dispersion le long de l'axe longitudinal du cours d'eau; b) il peut être découpé en un nombre quelconque de segments discrets (plans verticaux normaux à l'axe longitudinal) s'il le faut pour décrire la variation spatiale de la contamination chimique; c) il peut traiter le rejet instantané, continu ou variable dans le temps de déchets chimiques; d) il permet d'obtenir une description temporelle de la contamination du cours d'eau; et e) il tient compte des phénomènes d'adsorption et de désorption par la végétation et les sédiments de fond.

Introduction:

A chemical contamination, whether agricultural or domestic, municipal or industrial, cold or hot, when discharged into a stream, will mix and disperse according to turbulent flow characteristics of the stream. Presently, significant advances have been made in the understanding of the basic mechanism of dispersion, but the problem of predicting the time-concentration distribution of a water quality constituent still remains to be settled. The industrial wastes or radionuclides may enter the stream as soluble 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 chemical waste or radionuclides may undergo changes in state, remain in solution, or interact with various components of the aquatic system. Important factors that influence the contaminant concentration are: (a) the adsorption of each contaminant by bed sediments; (b) the adsorption of contaminant by aquatic plants; (c) the desorption of contamination into flowing water; (d) the migration of contamination through bed sediments; (e) the movement of sediment and attached radionuclides through normal movement of suspended sediment or bed sediments; (f) the period of contact and retention in the system, i.e. transport time associated with advection and dispersion.

The physical and chemical changes that occur in a typical stream environment can be measured, and while considerable attention has been directed to finding solutions to the phenomenon of dispersion and advection, bottom sediment transport, adsorption and desorption by the aquatic ecosystem etc., the development of a mathematical model that includes all of these factors.

Recognizing the need for a model to include interaction between the numerous factors

mentioned above, the primary objective of this study was to develop a simple mathematical model, in a form suitable for numerical simulation modelling, for routing a chemical waste or radionuclide contamination through a stream. To develop this model, several general requirements must be fulfilled. This model must have the following basic capabilities: (a) to treat advection and dispersive transfers of contamination along the longitudinal axis of a one-dimensional system; (b) to allow the channel to be discretized into elements of uniform length and cross-section (vertical planes normal to the longitudinal axis); (c) to be capable of receiving instantaneous, continuous, or varying release of chemical waste or radioactive contamination; (d) to provide for temporal description of the chemical waste or radionuclide activity throughout the system; and (e) to be capable of treating the following as source and/ or sinks:- (i) adsorption and desorption by bottom sediments, and (ii) sorption and desorption by aquatic plants.

Mathematical Model:

Many mathematical models (Booty and Lam, 1989) have been developed to describe the transport of various contaminants in fresh water ecosystems. The mathematical models usually assumed an eddy diffusivity mechanism. The basic transport equation can be written for a three dimensional system as:

$$dC/dt = d/dx\,(K_x\, dC/dx) + d/dy\,(K_y\, dC/dy) + d/dz\,(K_z\, dC/dz) - (u_x\, dC/dx + u_y\, dC/dy + u_z\, dC/dz) + S \qquad (1)$$

where, K_x, K_y and K_z are turbulent dispersion coefficients in the x,y, and z directions; u_x, u_y and u_z are fluid velocities in each of the coordinate directions; C is the concentration at any point

(x,y,z), t is the time and S is the source or sink.

The above equation states that changes in conservative substances are due to turbulent dispersion and convection in three directions. Equation (1) is complex and difficult for practical applications. Therefore, in numerous studies simplified versions of the equation were proposed to describe chemical waste or radionuclide contamination transport in one or two-dimensional equations. In order to simulate the uptake in regions of low velocity and by sediments and plants, other parameters were added to the equation. A transport function was derived by applying the sorption and desorption concepts to the mass balance principle.

A mathematical model for the transport of chemical waste or radionuclide contamination in an aquatic environment is:

$$dC/dt = D_L(d^2C/dx^2) - u(dC/dx) + \Sigma_{j=1}^{m} S_j \qquad (2)$$

where C is the concentration of chemical waste or a particular radionuclide contamination in the flowing stream at any point x, and time t; x is the distance in the direction of flow; D_L is the longitudinal dispersion coefficient; u is the average velocity of flow; S_j is uptake or release from the j th of m adsorption phases; and j is the index number for each adsorption phase. The first two terms in equation (2) define the mixing characteristics and dilution, while the third term describes uptake and release of contamination.

Sources and Sinks:

In general, the adsorption terms for plants and bottom sediments have the following form (Gloyna and Ledbetter, 1969; Gromiec and Matsui, 1978):

$$S_j = K_j[W_j - g_j(C)] \qquad (3)$$

where K_j is the mass transfer coefficient for phase j; $g_j(C)$ is the transfer function relating the concentration of activity in water to the equilibrium level in phase j, and W_j is the specific activity in the j th of m adsorption phases.

The activity in W_j is determined by:

$$dW_j/dt = K_j[g_j(C) - W_j] \qquad (4)$$

Usually the equilibrium concentration of chemical waste or radionuclide contamination in a sorbent, g(C), has the Freundlich isotherm form:

$$g(C) = K*C^n \qquad (5)$$

where K and n are constants pertaining to a given chemical waste or radionuclide contamination and adsorption phase. For uptake of most chemical waste or radionuclide contaminants n=1.0 and K becomes Kd, the equilibrium distribution coefficient. Thus, the non-equilibrium chemical waste or radionuclide contaminant adsorption reaction with a given material is derived as:

$$dW_j/dt = K_j[Kd_jC - W_j] \qquad (6)$$

and it follows that,

$$S_j = K_j[W_j - Kd_jC] \qquad (7)$$

Numerical Solution:

Once the initial and boundary conditions are specified, the boundary value problem can be solved to obtain C(x,t). However, the nonlinear partial differential equation can not be solved analytically except perhaps for trivial geometries. Therefore, numerical techniques have to be

resorted to for solving the mass transport problems. These techniques usually transform the partial differential equations of the mass transport system into systems of ordinary differential or algebraic equations. The solution of these equations determines the values of the dependent variables at a predetermined set of discrete nodal points within the flow domain. The finite difference methods are widely used for solution of the mass transport equations (Lam and Simpson, 1976; Bobba and Bukata, 1980). The main advantage of the finite difference methods is that they reduce the differential equations to algebraic equations which can be solved much more easily compared to their parent differential equations. In finite difference methods, the partial derivatives such as dC/dx in the governing mass flow equations are replaced by the differences $\Delta c/\Delta x$. The solution domain is first divided into a set of grids formed by lines representing space and time. The finite difference equations use the distance between grid points as the increments for the independent variables in respective directions which in turn form the denominators for the difference approximation of the derivatives. The set of finite difference equations thus obtained are solved numerically on a digital computer, which results in the values of the dependent variables at the predetermined grid points.

There are two broad classes of finite difference solution schemes, namely the **explicit** scheme and the **implicit** scheme. In an explicit scheme, one can solve for dependent variable, C, at some grid point (nodal point), for time $t+\Delta t$ from the knowledge of C at the preceding time, t, corresponding to the neighbouring grid (nodal) points. Therefore, the determination of a nodal dependent function at some time is independent of dependent function values at other nodes for the same time. In an **implicit** scheme the dependent function value at a particular node at some time depends on the function values at its adjoining nodes for the same time, which is in general

unknown. Therefore, to determine the unknown nodal function values at t+Δt, one is forced to solve all nodal equations corresponding to the time t+Δt simultaneously; and a single value of the dependent variable at a particular node cannot be computed explicitly at time t+Δt. The complete solution would then require simultaneously solving the nodal equations at each time t+Δt, t+2Δt,...until the specified final time is reached.

Since the mass transport 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*h and t= n*e, where i = 1,2,....I and n= 0,1,2..N. The concentration, C, at each mesh point is approximated by C(i*h, n*e) which is denoted by C^n_i. By applying the implicit method in which derivatives are approximated by expanding C^n_i in a Taylor series and averaging over the time step, e, the contaminant transport equation may be written as:

$$R_1 = 0.5 * D_L [R_2 + R_3] - 0.5 * u[R_4 + R_5] \quad (8)$$

where,

$$R_1 = (C_i^{n+1} - C_i^n)/e$$

$$R_2 = (C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1})/h^2$$

$$R_3 = (C_{i+1}^{n} - 2C_i^{n} + C_{i-1}^{n})/h^2$$

$$R_4 = (C_{i+1}^{n+1} - C_{i-1}^{n+1})/2h$$

$$R_5 = (C_{i+1}^{n} - C_{i-1}^{n})/2h$$

and, i= 1,2, ...I, and n= 0,1,2,...N. The details of the numerical method has been presented by Smith (1965) and Remson et.al (1970). The boundary conditions for **instantaneous** release are:

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

$C_i^n = 0$; as i----> ∞

C_i^n = finite value as n ---->∞

and the **initial condition** is:

$$C_0^{t+t_0} = Q_1 * Q_2 \quad (9)$$

where,

$Q_1 = M/A*[4.0 * \pi * D_L (t+t_0)]^{0.5}$,

$Q_2 = \exp\{-[u (t+t_0)]^2/ [4.0*\pi*D_L (t+t_0)]\}$

where, t_0 is a time slightly greater than zero for which a finite solution for the equation can be obtained. For a **continuous release,** the boundary condition is:

$$C_0^n = M/QT \quad (10)$$

for all n where T is the time span over which the continuous release occurs. Equation (8) may also be expressed as:

$$a*C_{i-1}^{n+1}+ b*C_i^{n+1}+ c*C_{i+1}^{n+1}= (D_L*e)/(2h^2)*Y_1-(u*e)/(4h)* Y_2+C_i^n \quad (11)$$

where $Y_1 = (C_{i+1}^n-2C_i^n+C_{i-1}^n)$

$Y_2 = (C_{i+1}^n-C_{i-1}^n)$

$Y_3 = (W_{j,i}^n-Kd_j*C_i^n)$

$$a = -(D_L*e)/(2h^2)-(u*e)/(4h) \quad (12)$$

$$b = 1+(D_L*e)/h^2 \quad (13)$$

$$c = -(D_L*e)/(2h^2)+(u*e)/4h \quad (14)$$

The mass transport equation, Eq (11) with adsorption terms,becomes:

$$a*C_{i-1}^{n+1}+b*C_i^{n+1}+c*C_{i+1}^{n+1} = (D_L*e) / (2h^2)*Y_1-(u*e) / (4h)*Y_2 + e\Sigma^m_{j=1} K_j*Y_3 \quad (15)$$

Bottom Sediments:

For bottom sediments, the mass transport equation can be expressed in the following form (Gloyna and Ledbetter, 1969; Gromiec and Matsui, 1978):

$$dW_{1,i}/dt = K_1[Kd_1 * C_i - W_{1,i}] \quad (16)$$

and Equation (7) can be expressed as:

$$S_{1,i}= (K_1/H * A_{cs}) [W_{1,i} - Kd_1 C_i] \quad (17)$$

where A_{cs} is the cross sectional area of a sediment sample, and H is an effective depth of sediments.

In finite-difference form, Equation (16) and Equation (17) become:

$$W_{1,i}^{n}= W_{1,i}^{n-1} + e*K_1[Kd_1C_i^{n-1} - W_{1,i}^{n-1}] \quad (18)$$

and

$$S_{1,i} = (K_1 / HA_{cs}) [W_{1,i}^{n} - Kd_1C_i^{n}] \quad (19)$$

Vegetation:

For vegetation, the mass transport equation is used in a similar fashion as in Equation (16) and Equation (17), and in finite difference form as:

$$W_{2,i}^{n} = W_{2,i}^{n-1} + e*K_2[Kd_2C_i^{n-1} - W_{2,i}^{n-1}] \quad (20)$$

and

$$S_{2,i}^{n} = M_bK_2 [W_{2,i}^{n} - Kd_2 C_i^{n}] \quad (21)$$

where M_b is biomass of vegetation.

With the adsorption terms for bottom sediments and vegetation included, Equation (15) becomes:

$$a*C_{i-1}^{n+1}+b*C_i^{n+1}+c*C_{i+1}^{n+1} = (D_L*e/2h^2)*Z_1-(u*e/4h)*Z_2+(K_1*e/H*A_{cs})*Z_3+ M_b*e*K_2 * Z_4 \quad (22)$$

where,

$Z_1 = (C_{i+1}^n - 2C_i^n + C_{i-1}^n)$

$Z_2 = (C_{i+1}^n - C_{i-1}^n)$

$Z_3 = (W_{1,i}^n - Kd_1\ C_i^n)$

$z_4 = (W_{2,i}^n - Kd_2\ C_i^n)$

$i = 1,2,.... I$ and

$n = 0,1,2....N$

If Equation (22) is rewritten at some point in time, n, for all values of i, in matrix notation it becomes A*C = d, (see,appendex 1, where A represents the coefficient matrix, C represents the column matrix of unknowns, and d represents the column matrix of known quantities. The matrix [A] is tridiagonal since any row excluding the top and bottom rows contains only three terms, the diagonal and immediately adjoining off diagonal terms. The bottom and top rows which express the boundary conditions contain the diagonal and one off diagonal term (Remson et.al.1970). The equation (23) can be solved by a number of different methods but for this case the equation is solved by the method described by Ralston and Wilf (1967).

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:

(a) Set $f_1 = c_1/b_1$ and $g_1 = d_1/b_1$

(b) Then operate from row 2 to the last row, I, using the recursive relations below for i = 2, I. Compute

$$f_i = c_i /(b_i - a_i f_{i-1})$$

$$g_i = (d_i - a_i g_{i-1})/(b_i - a_i f_{i-1})$$

and store these quantities since:

$$C_i^{n+1} = g_i - f_i C_{i+1}^{n+1} \qquad (24)$$

The last row, I, is such that

$$C_I^{n+1} = g_i$$

(c) With C_I^{n+1} computed, operate with equation (24) from row I-1 to row 1, i.e., back substitution. The back substitution yields the set of concentration, C_i^{n+1}, to advance the solution over the time step e.

Model Capability:

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

a) It distributes chemical waste concentration or radionuclide activity by advective and dispersional mechanisms along the longitudinal axis of the system.

b) 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 chemical waste concentration or radionuclide activity.

c) It is capable of treating instaneous, continuous, or time varying releases of chemical contamination or radionuclide activity.

d) It provides for a temporal description of chemical waste or radionuclide activity throughout the system.

e) It provides for adsorption and desorption by both vegetation and bottom sediments.

Application of the Model:

The model has been applied to a hypothetical stream. The shapes of the contaminant curves are shown in Figure 1, at different locations in the stream. From the shape and maximum values of the calculated data, it can be seen that initial dispersion of a point source does not follow Taylor's Equation (2), but rather takes the shape of a skewed normal distribution because of dominance of convection over dispersion. However, at some point downstream, the curves approach a form where the Taylor expression is valid.

The results obtained with an adsorption term for bottom sediments added to the dispersion equation are shown in Figure 2. Continuous release of contamination may also be modeled with this solution. The transport equation with adsorption terms for bottom sediments and vegetation was used for the continuous release case and the results are shown in Figure 3.

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 chemical waste or radionuclide activity. If flows are steady and the geometric properties rather uniform from

place to place, it is sufficient to present the system with a few prismatic segments of a fixed geometry. The length of channel segment depends, in such cases, more on the variations of input data than on flow or cross section configuration, with the optimum length being chosen to provide the necessary detail required to describe the chemical waste or radionuclide activity along the axis of flow.

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 streams wide variation in geometry may be expected along the axis of flow and the effects of these on dispersion and advection transport may be further magnified by the inherent unsteadiness in natural flows. Consequently, in such cases, a satisfactory description of the chemical waste or radionuclide transport will probably require maximum detail. This might entail a need to look at two-dimensional modelling, 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 chemical waste or radionuclides associated with the liquid phase

and various solid phases, i.e., the vegetation, the bottom sediments, and suspended particles, etc., of a stream may produce a significant effect on the net transport of chemical waste or radionuclides. These components or adsorption 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 vegetation, types of sediments, and sediment transport characteristics of a natural stream will be required.

Data Requirements:

The following brief discussion presents the data requirements for what may be regarded as a normal stream simulation problem.

a)Hydraulic data:

1) For steady flow: Water surface area of each channel segment. Length and cross-sectional area of each channel segment.

2) For unsteady flow: Depth-surface area curve for each channel segment. Length and depth-cross-sectional area curve for each channel segment.

3) Longitudinal dispersion: velocity profiles, roughness, and sinuosity of stream.

4) Waste discharge: amount, quality, and location.

5) Tributary inflows: amount, quality, and location.

b) Chemical Waste Data:

1) Detailed description of release conditions and amount released.

2) Spatial and temporal description of chemical waste after release. This will require a comprehensive sampling program throughout the stream 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.

c) Environmental Data:

1) Detailed description of the biota throughout the stream system.

2) Detailed description of the bottom sediments throughout the stream system.

3) Detailed description of the sediment transport characteristics throughout the stream system.

Conclusions:

A mathematical model has been developed for routing the chemical waste contamination through a small stream system. The capabilities of this simulation model include the following characteristics: a) It distributes contamination by advection and dispersion along the longitudinal axis of the system. b) 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 chemical contamination. c) It is capable of treating instantaneous, continuous, or time varying releases of radionuclide activity. d) It provides for temporal description of contamination throughout the system. e) It provides for sorption and desorption by both vegetation and bottom sediments.

Acknowledgments:

The encouragement and support from E.D. Ongley and R.L. Thomas are also appreciated.

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APPENDIX 1

$$
\begin{bmatrix}
b_1 & c_1 & & & & \\
a_2 & b_2 & c_2 & & & \\
 & a_3 & b_3 & c_3 & & \\
 & & \cdot & & & \\
 & & & \cdot & & \\
 & & & & c_{I-1} & \\
 & & & a_I & b_I &
\end{bmatrix}
\begin{bmatrix}
C_1^{n+1} \\
C_2^{n+1} \\
C_3^{n+1} \\
\cdot \\
\cdot \\
C_{I-1}^{n+1} \\
C_I^{n+1}
\end{bmatrix}
=
\begin{bmatrix}
d_1 \\
d_2 \\
d_3 \\
\cdot \\
\cdot \\
d_{I-1} \\
d_I
\end{bmatrix}
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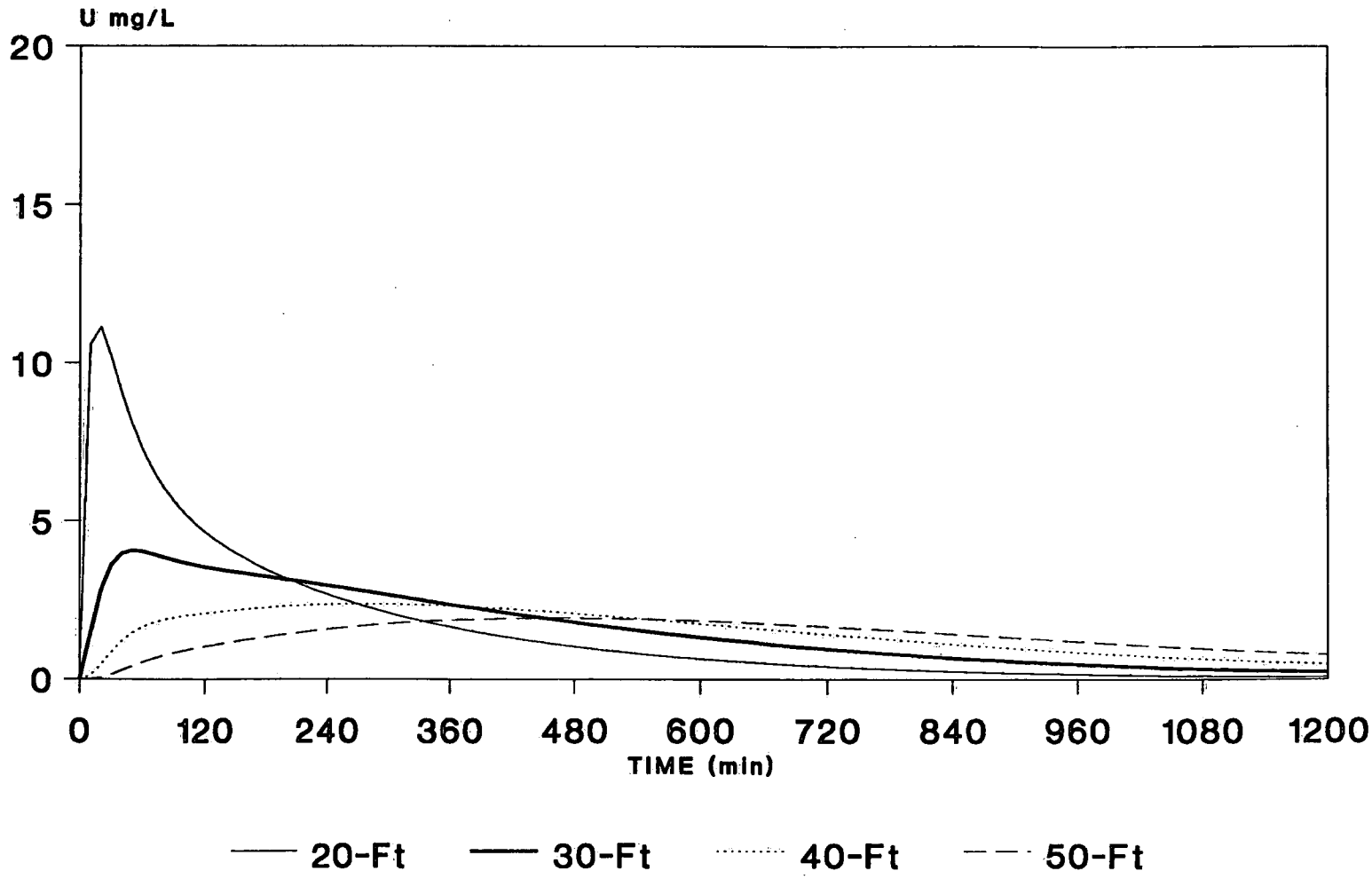
STREAM CONTAMINATION MODEL
RADIOACTIVE



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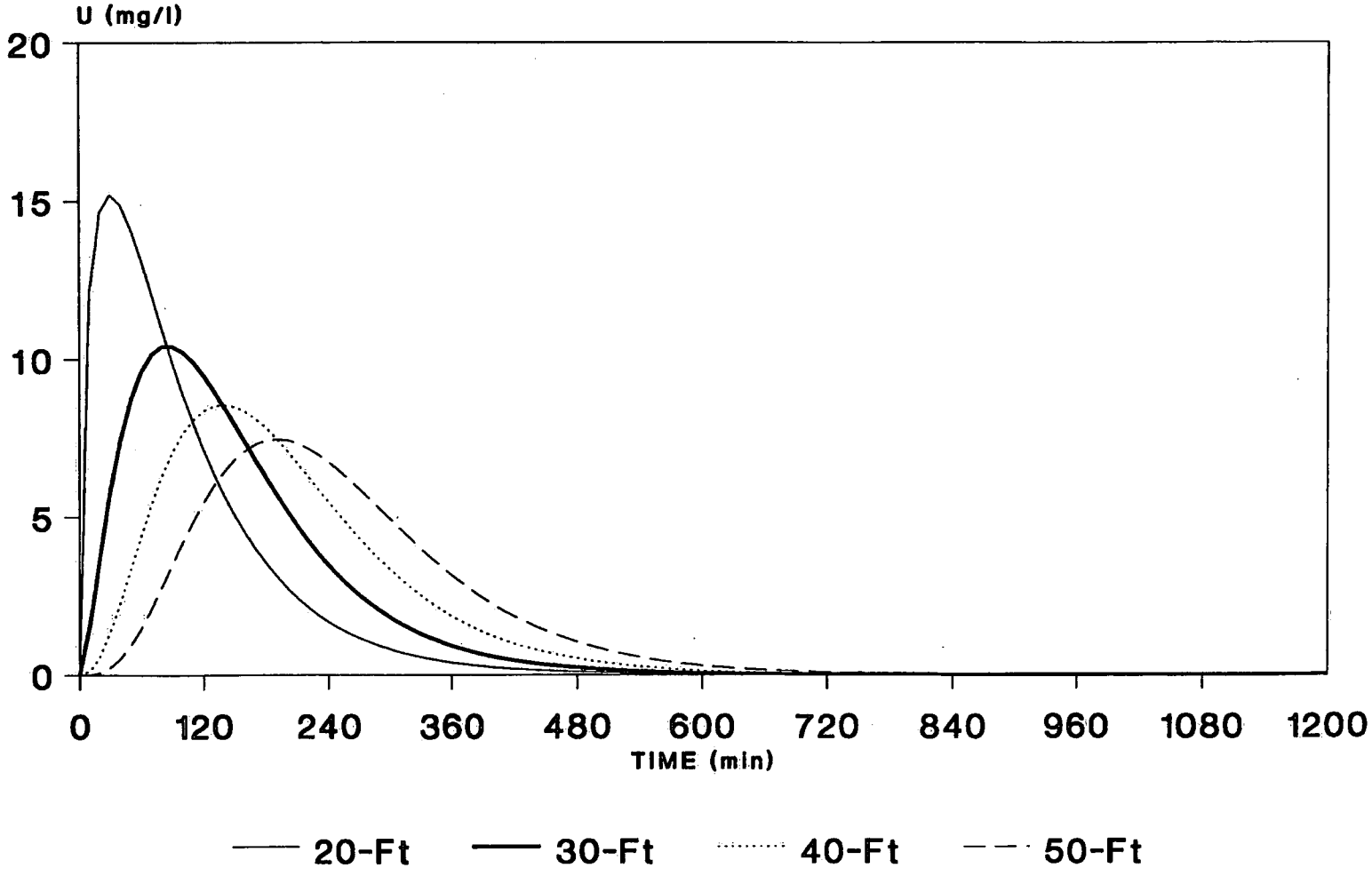
RADIOACTIVE



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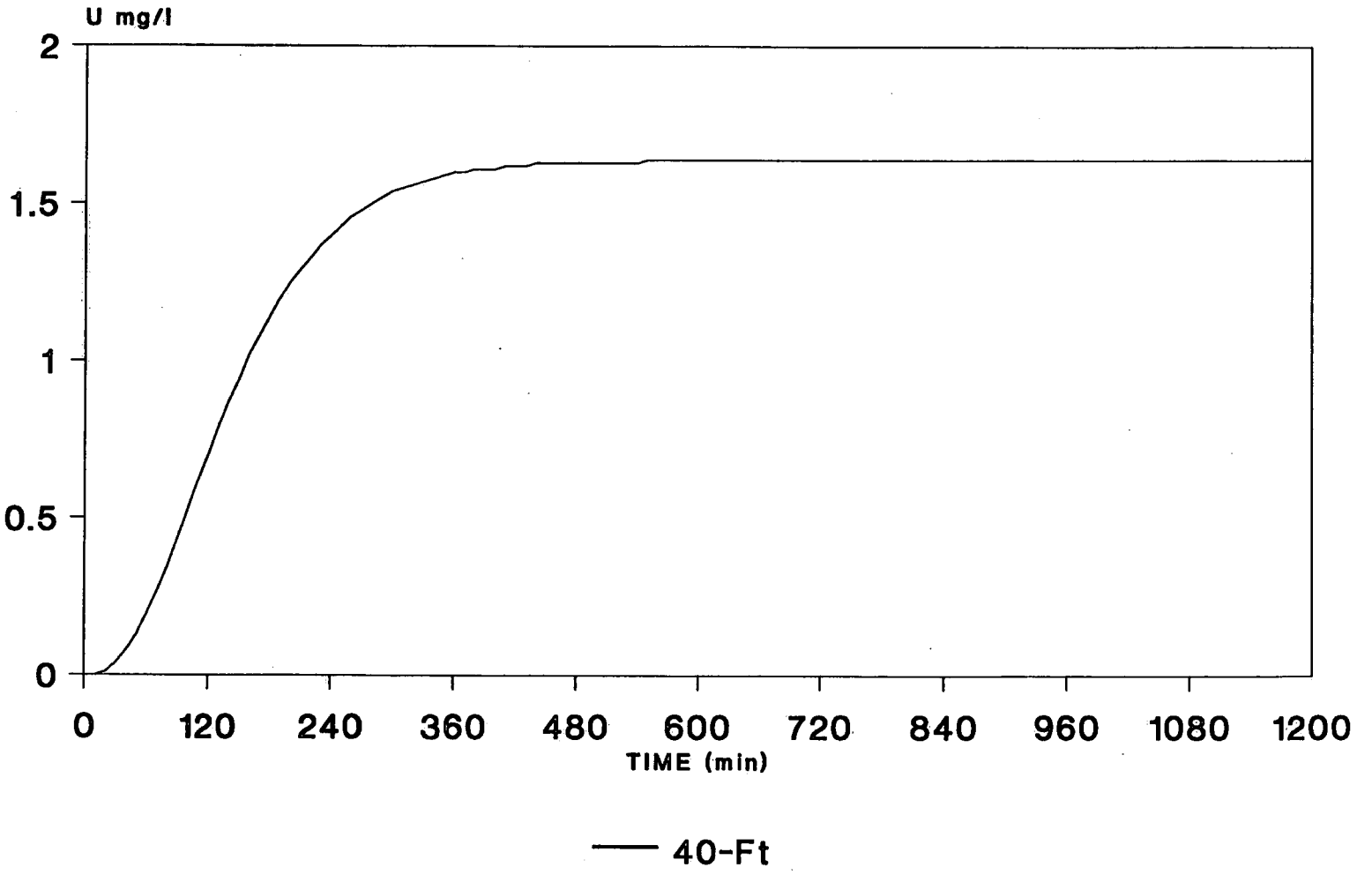
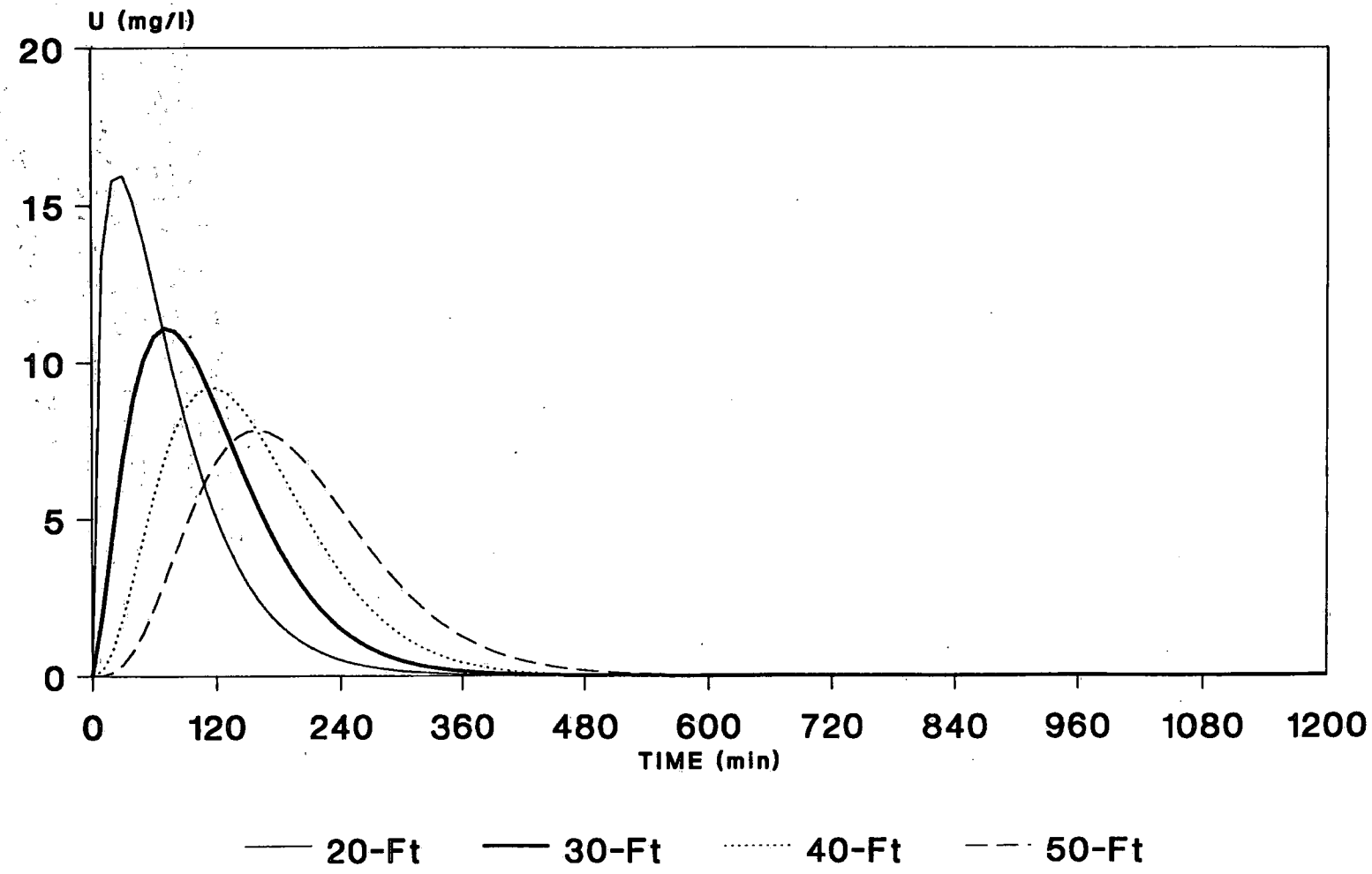


CONTINUOUS

STREAM CONTAMINATION MODEL
RADIOACTIVE



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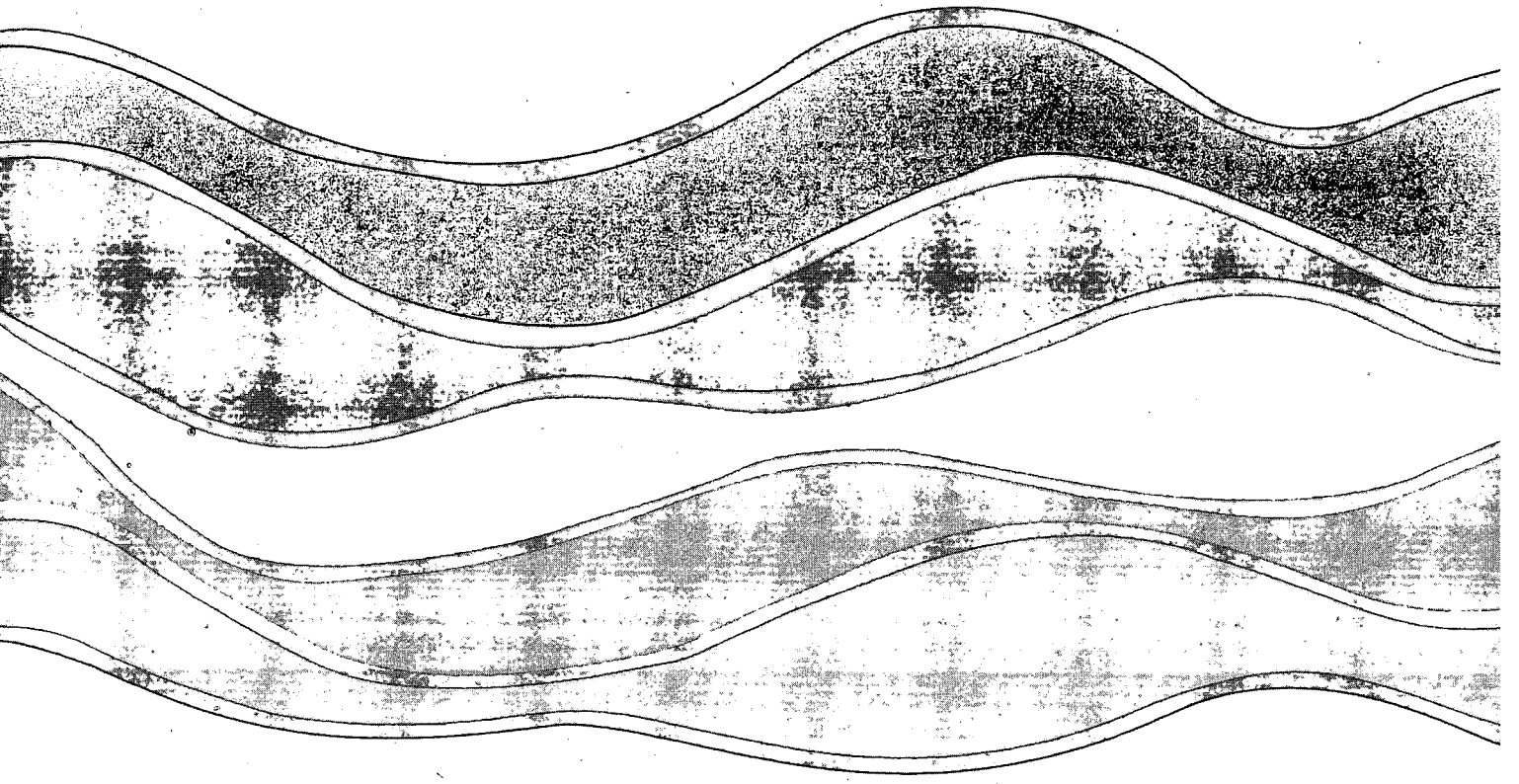

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P.O. BOX 5050, BURLINGTON, ONTARIO L7R 4A6

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C.P. 5050, BURLINGTON (ONTARIO) L7R 4A6