NUREG/CR-0658

PNL-2902

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**Annual Report
October 1977 to September 1978**

**Mathematical Simulation
of Sediment and Contaminant
Transport in Surface Waters**

January 1979

**Prepared for
the U.S. Nuclear Regulatory Commission**

**Pacific Northwest Laboratory
Operated for the U.S. Department of Energy
by Battelle Memorial Institute**

PNL-2902

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PACIFIC NORTHWEST LABORATORY
operated by
BATTELLE
for the
UNITED STATES DEPARTMENT OF ENERGY
Under Contract EY-76-C-06-1830

Printed in the United States of America
Available from
National Technical Information Service
United States Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22151

Price: Printed Copy \$ ____*; Microfiche \$3.00

*Pages	NTIS Selling Price
001-025	\$4.00
026-050	\$4.50
051-075	\$5.25
076-100	\$6.00
101-125	\$6.50
126-150	\$7.25
151-175	\$8.00
176-200	\$9.00
201-225	\$9.25
226-250	\$9.50
251-275	\$10.75
276-300	\$11.00

NUREG/CR-0658
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ANNUAL REPORT
OCTOBER 1977 TO SEPTEMBER 1978

MATHEMATICAL SIMULATION OF SEDIMENT AND
CONTAMINANT TRANSPORT IN SURFACE WATERS

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January 1979

Prepared for
the U.S. Nuclear Regulatory Commission
under a Related Services Agreement
with the U.S. Department of Energy
Contract EY-76-C-06-1830
FIN No. B2271-9

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LIST OF SYMBOLS

- A = the river bed surface area
- a = unit conversion constant in Equation 3.35
- a' = an empirical constant (≈ 0.6)
- a_j = wave amplitude
- A_0 = constant used in Equation 3.20
- B = width of the river
- B^* = coefficient used in Equation 3.19
- C_j = concentration of sediment of j^{th} type (weight of sediment per unit volume of water)
- $\bar{C}_j$ = depth averaged concentration of sediment for j^{th} type
- c_j'' = fluctuations from the depth averaged concentration of sediment of j^{th} type
- C_0 = bed load concentration in Equation 3.20
- D = equivalent sediment particle diameter
- D_{xj}, D_{yj} = dispersion coefficients of x and y directions for j^{th} sediment type
- D_{xw}, D_{yw} = dispersion coefficients of x and y directions for a dissolved contaminant
- E_b = the energy of the breaking waves
- $(ECn)_b$ = the energy flux of the waves evaluated at the breaker zone
- f_{sj} = fraction of contaminant sorbed by j^{th} sediment
- f_w = fraction of contaminant left in solution
- g = gravitational acceleration
- G_{bj} = particulate contaminant concentration associated with j^{th} sediment in river bed
- G_j = particulate contaminant concentration associated with j^{th} sediment (weight of contaminant per unit weight of sediment)

G_w = dissolved contaminant concentration (weight of contaminant per unit volume of water)
 $\bar{G}_w$ = depth averaged value of pollutant concentration
 G_w'' = fluctuation from the depth averaged value of pollutant concentration
 h = flow depth
 h_b = water depth at wave breaking
 I_ℓ = immersed weight littoral transport rate
 K_{dj} = distribution (or partition) coefficient between dissolved contaminant and particulate contaminant associated with j^{th} sediment
 K_j = wave number
 K_j = transfer rate of contaminant for j^{th} sediment
 K_j' = an empirical constant depending on the sediment type
 $K_{xj} = \epsilon_{xj} + D_{xj}$
 $K_{yj} = \epsilon_{yj} + D_{yj}$
 $k_{xw} = \epsilon_{xw} + D_{xw}$
 $k_{yw} = \epsilon_{yw} + D_{yw}$
 M_j = erodibility coefficient for sediment of j^{th} type fraction
 M_j' = weight of j^{th} sediment
 P = probability
 Q_{aT} = actual total sediment load
 Q_B = bed load
 Q_S = suspended load
 Q_T = sediment transport capacity of flow
 S_{Dj} = sediment deposition rate per unit bed surface area for j^{th} sediment type

- S_L = volumetric littoral transport
- S_{Rj} = sediment erosion rate per unit bed surface area for j^{th} sediment type
- t = time
- U = velocity component of longitudinal (x) direction
- $\bar{U}$ = depth averaged longitudinal velocity
- $\bar{u}$ = average horizontal velocity in the boundary layer calculated by Equation 3.21
- u'' = longitudinal velocity fluctuation from the depth averaged longitudinal velocity
- U_{AB} = velocity component of incidental flow (other than that induced by a wave action) near the ocean bed
- U_B = mass transport velocity (second order velocity components) of a wave near the ocean bed
- U_I = velocity of incidental flow (other than that induced by waves) in a surf zone, and
- U_{IS} = velocity component of incidental flow (other than that induced by wave action) in the interior zone
- U_S = mass transport velocity (second order velocity component) of a wave in the interior zone
- V = velocity component of lateral (y) direction
- $\bar{V}$ = depth averaged lateral velocity
- v'' = lateral velocity fluctuation from the depth averaged lateral velocity
- $\bar{v}_L$ = velocity caused by the combination of waves and currents in a surf zone
- W = velocity component of vertical (z) direction
- W_{sj} = fall velocity of sediment particle of j^{th} type
- x, y, z = longitudinal, lateral and vertical direction in Cartesian coordinates, respectively

α_b = wave breaker angle with the shoreline

γ = coefficients used in Equations 3.3 and 3.4

γ_s = specific weight of sediment

$\epsilon_{xj}, \epsilon_{yj}, \epsilon_{zj}$ = diffusion coefficients of longitudinal, lateral and vertical directions for j^{th} sediment type

$\epsilon_{xw}, \epsilon_{yw}, \epsilon_{zw}$ = longitudinal, lateral and vertical diffusion coefficients for dissolved contaminant

ζ_0 = coefficient used in Equation 3.19

λ = chemical and biological decay rate of contaminant

ρ = water density

ρ_s = sediment density

σ = constant shown in Equation 3.24

τ_b = bed shear stress

τ_c = critical bed shear stress used in the DuBoys's formula (Equation 3.13)

τ_{cdj} = critical shear stress for sediment deposition for j^{th} sediment type fraction

τ_{crj} = critical shear stress for sediment erosion for j^{th} sediment type fraction

ν = kinematic viscosity of water

ψ = nondimensional bed shear stress used in Equation 3.19

ψ_D = coefficient used in the DuBoys's formula (Equation 3.13)

ω_i = wave frequency

1. INTRODUCTION

The nuclear energy industry has grown considerably during the past decade, and nuclear power is expected to become one of the major sources of energy to meet growing needs. Although considerable effort is being made to minimize the release of the radioactive wastes into the environment, it is important to assess the potential environmental impact of radionuclide releases. Various pathways exist for exposure of humans and biota to radioactive materials released from nuclear facilities. Hydrologic transport (liquid pathway) is one element in the evaluation of the total radiation dose to man. Exposures can occur from routine or accidental releases of radionuclides in liquid effluents from nuclear facilities. Mathematical models supported by well-planned field data collection programs can be useful tools in assessing the hydrologic transport and ultimate fate of radionuclides.

Many radionuclides found in surface waters originated from effluents discharged from nuclear power plants, waste burial sites and other nuclear-related facilities. These radionuclides are dispensed by stream flows, ocean currents, surface waves and turbulent mixing. However, radionuclides with high distribution coefficients (e.g., cerium, cesium, plutonium) or radionuclides in surface waters with high suspended sediment concentrations are, to a great extent, adsorbed by river and marine sediments. Thus, otherwise dilute contaminants are concentrated. Contaminated sediments may be deposited on the river and ocean beds creating a significant pathway to man. Contaminated bed sediment in turn may become a long-term source of pollution through desorption and resuspension. In contrast, sorption by sediment can be an important mechanism for reducing the area of influence of these contaminants by reducing concentrations of dissolved constituents.

Field measurements⁽¹⁾ of radionuclide concentrations in the Clinch River indicate that approximately 90% of the ^{137}Cs released was adsorbed by the suspended sediment in the river within 20 miles downstream from the effluent discharge. Measurements conducted in the Irish Sea near the Wildscale Nuclear Fuel Reprocessing Plant in England indicate that approximately 95% of the plutonium discharged from the plant to the Irish Sea

was adsorbed by marine sediment and only 5% remains in solution in sea water.⁽²⁾ These data also revealed that ^{106}Ru and ^{144}Ce behave in a manner similar to ^{239}Pu . At the other extreme, most of the ^3H and ^{90}Sr are expected to be in a dissolved form.

In order to assess migration and accumulation of radionuclides in surface waters, mathematical models must correctly simulate essential mechanisms of radionuclide transport. Currently numerous mathematical models ranging from very simple analytical methods to sophisticated numerical models are available that may or may not be applicable to specific surface waters.⁽³⁻⁵⁾ For example, mathematical models that calculate radionuclide transport without including the radionuclide-sediment interaction predict that radionuclides will be flushed from surface waters at the same rate at which water is exchanged. In reality, however, sediment sorption effects would cause some radionuclides to flush much more slowly, at approximately the rate at which the sediment is exchanged in the surface water system. Hence, in some cases, neglecting these sediment effects prohibits accurate prediction of radionuclide migration.⁽⁴⁾

The objective of this study for FY1978 were:

1. to conduct a critical review of
 - (a) radionuclide transport models as well as sediment transport and representative water quality models in rivers, estuaries, oceans, lakes and reservoirs, and
 - (b) adsorption and desorption mechanisms of radionuclides with sediments in surface waters
2. to synthesize a mathematical model capable of predicting short- and long-term transport and accumulation of radionuclides in marine environments.

2. LITERATURE SURVEY ON TRANSPORT MODELING AND SORPTION MECHANISMS OF RADIONUCLIDES

Both published and unpublished information was critically reviewed to evaluate the state-of-the-art of mathematical modeling of radionuclide transport in surface waters, and current knowledge on adsorption and desorption mechanisms of radionuclides with sediments in surface waters. For supplemental information, sediment transport and representative water quality models were evaluated to determine if these models, with some model modifications, could be used to predict radionuclide migration and accumulation.

This comprehensive review work was completed and a draft topical report for this subject was submitted to NRC in May 1978. The final topical report will be submitted to NRC in early 1979. The report is entitled "Critical Review: Radionuclide Transport, Sediment Transport and Water Quality Mathematical Modeling and Radionuclide Sorption/Desorption Mechanisms" NUREG-CR-0657/PNL-2901 by Y. Onishi, R. J. Serne, E. M. Arnold, C. E. Cowan, and F. L. Thompson.

The report discusses almost all available radionuclide transport models for oceans, estuaries, rivers, lakes and reservoirs. There are many dissolved radionuclide transport models, mostly applicable to rivers, and only a limited number of models applicable to oceans, estuaries and impoundments. Even fewer models are found to solve both dissolved and particulate radionuclides, e.g., Gloyne et al.,⁽⁶⁻¹⁰⁾ Onishi,^(5,11-13) Field.⁽¹⁴⁾ Models developed by Onishi et al. and Field are the only ones that simulate both dissolved and particulate radionuclide transport by including sediment-radionuclide dynamic interactions. Eraslan's model⁽¹⁵⁾ (Unified Transport Application model developed by ORNL) was not fully evaluated because the detailed formulations of this model (series of transport models of heat, chemicals, radionuclides and aquatic biota) are not yet published.

Because there is a very limited number of available radionuclide models for surface waters, a review was also made of water quality and sediment transport models to evaluate if any of these models can be modified for

radionuclide transport. Since there are many of these models, especially water quality models, these models were divided into several groups based on their model formulations or physical characteristics. Several representative models for each group were then reviewed for their model description and their applicability to the radionuclide transport. The evaluation of these models is as follows: Most of the water quality models can simulate dissolved radionuclide transport with only a minor modification; however, extensive modifications will be required for these models to calculate particulate radionuclide transport as well. Sediment transport models, on the other hand, can simulate particulate radionuclide movement fairly well with some model modification. Nonetheless, it will be a major task to handle both dissolved and particulate radionuclide including sediment interactions.

Exhaustive numbers of reports and papers were also critically reviewed to identify the present knowledge on radionuclide adsorption/desorption mechanisms, especially interaction with sediment in surface waters. Because of their importance, Am, Sb, Ce, Cs, Co, Cm, Eu, I, Np, Pu, Pm, Ra, Ru, Sr, Tc, Th, ^3H , U and Zr are discussed in detail in the topical report. Functional relationship between K_d and various parameters (e.g., sediment size and type, water quality parameters) is discussed. Also, most available values of K_d for these radionuclides are compiled in a tabular form. Although there is much work conducted for K_d , there is almost no functional relationship developed between K_d and the various parameters.

The literature search revealed that:

1. Except for a few, almost all models deal with only dissolved radionuclide transport.
2. Sediment-contaminant transport models, SERATRA^(5,11) and FETRA⁽¹¹⁻¹³⁾ developed by Onishi et al., CHNSED⁽¹⁴⁾ developed by Field, and UTA⁽¹⁵⁾ being developed by Eraslan et al., are the most advanced computer codes to solve radionuclide transport including sediment-radionuclide interactions (radionuclide adsorption and desorption, transport, deposition and resuspension of contaminated sediment, etc.).
3. Knowledge on radionuclide adsorption/desorption mechanisms is still very limited.

3. SYNTHESIS OF RADIONUCLIDE TRANSPORT MODELS FOR OCEANS

Based on the literature survey, a mathematical model capable of predicting migration and accumulation of radionuclides in marine environments was synthesized from available models. A topical report for this study is under preparation.

SELECTION OF MODELS

For the purpose of selecting one or more models from those reviewed to be applied to oceans and the Great Lakes, the following criteria were used:

1. The model should provide a numerical solution of some form of the advection-diffusion equations.
2. The model should be at least two-dimensional (longitudinal and lateral directions).
3. The models should be able to simulate the transport of radionuclide species present in oceans and the Great Lakes.
4. The selected models should have a documented history of success.

Of the two- or quasi three-dimensional models of radionuclide transport, sediment transport and water quality parameters reviewed, the models of Leendertse,^(16,17) Eraslan,⁽¹⁵⁾ DPRW,⁽¹⁸⁾ and FETRA,⁽¹¹⁻¹³⁾ are suitable for dissolved radionuclide transport. Thus, these models can simulate the movement of radionuclides with small distribution coefficients, e.g., ^3H , ^{90}Sr and ^{131}I which are mostly in a dissolved form. The nuclides with large distribution coefficients, e.g., ^{144}Ce , ^{137}Cs , $^{238,239,240}\text{Pu}$, ^{106}Ru and ^{95}Zr are present in both dissolved and suspended sediment-bound forms in surface waters. Of the remaining models studied, sediment transport models developed by Ariathurai et al.⁽¹⁹⁾ and Leimkuhler et al.⁽²⁰⁾ could simulate particulate radionuclide transport with fairly extensive modifications, but FETRA is the only available model that is applicable to both dissolved and particulate radionuclide transport. Thus, FETRA is the only available model capable of predicting the movement of all the radionuclide species in oceans and the Great Lakes.

After examining the candidate models with respect to the above criteria, the FETRA code was selected for modeling the transport of radionuclides in marine environments.

MODIFIED SEDIMENT AND CONTAMINANT TRANSPORT MODEL, FETRA

FETRA was originally developed for rivers and then extended to estuaries. Although the FETRA code is presently the most advanced model to calculate sediment and contaminant transport by including the effects of sediment-contaminant interaction,⁽⁴⁾ it has not been extended to ocean environments. FETRA must be modified when it is applied to oceans and the Great Lakes. Specifically, wave-sediment interaction must be included in the model. In ocean environments, marine sediments are suspended by waves which themselves can transport a very little amount of suspended sediment. The marine sediments suspended by wave actions are then transported by currents which, in most cases, are too small to suspend sediment without wave actions. Dissolved and particulate contaminant submodels of FETRA can be applied to ocean environments without any modification.

Another important aspect to be considered is the compatibility of FETRA to a hydrodynamic model which provides velocity field input data to FETRA. For marine environments, it is necessary to obtain unsteady, two-dimensional (longitudinal and lateral directions) radionuclide distributions which require unsteady, two-dimensional distributions of flow, depth and velocity. From the standpoint of compatibility to FETRA, these hydrodynamic distributions can best be obtained by the unsteady, two-dimensional, finite element model, RMA II, developed by Norton and King.^(21,22) However, some care must be taken to ensure the compatibility between FETRA and RMA II.

Mathematical Model Formulation of Modified FETRA

The modified FETRA code is an unsteady (as well as steady), two-dimensional finite element model, utilizing the Galerkin weighted residual method. The model consists of three submodels coupled to include the effects of sediment-contaminant interaction on contaminant transport. The submodels are: 1) sediment transport model, 2) dissolved contaminant transport model, and 3) particulate contaminant (contaminant adsorbed by sediment) transport model.

Sediment Transport Model

The sediment transport model solves the migration of sediment (transport, deposition and scouring) for three sediment size fractions (e.g., sand, silt and clay) separately, since movements and adsorption capacity vary significantly with sediment sizes. The model includes the effects of:

1. convection and dispersion of materials
2. surface waves to suspend sediments
3. fall velocity and cohesiveness
4. deposition on the river bed
5. resuspension from the river and ocean beds (bed erosion and armoring)
6. sediment contributions from tributaries.

Sediment mineralogy and water quality effects are implicitly included through the above mentioned effects 3, 4 and 5.

This model also calculates changes in river and ocean bed conditions, including bed elevation changes and distribution of the ratio of each sediment size fraction within the bed.

The governing equation of sediment transport for the three-dimensional case is:

$$\begin{aligned} & \frac{\partial C_j}{\partial t} + \frac{\partial}{\partial x}(UC_j) + \frac{\partial}{\partial y}(VC_j) + \frac{\partial}{\partial z} \left\{ (W - W_{sj})C_j \right\} \\ &= \frac{\partial}{\partial x} \left(\epsilon_x \frac{\partial C_j}{\partial x} \right) + \frac{\partial}{\partial y} \left(\epsilon_y \frac{\partial C_j}{\partial y} \right) + \frac{\partial}{\partial z} \left(\epsilon_z \frac{\partial C_j}{\partial z} \right) \end{aligned} \quad (3.1)$$

where

C_j = concentration of sediment of j^{th} size fraction (weight of sediment per unit volume of water)

t = time

U = velocity component of longitudinal (x) direction

V = velocity component of lateral (y) direction

W = velocity component of vertical (z) direction

W_{sj} = fall velocity of sediment particle of j^{th} type

x, y, z = longitudinal, lateral and vertical direction in Cartesian coordinates, respectively

$\epsilon_x, \epsilon_y, \epsilon_z$ = diffusion coefficients of longitudinal, lateral and vertical directions.

Boundary conditions are:

$$(W - W_{s_j})C_j - \epsilon_z \frac{\partial C_j}{\partial z} = 0 \quad \text{at } z = h \quad (3.2)$$

$$(1-\gamma) W_{s_j} C_j + \epsilon_z \frac{\partial C_j}{\partial z} = S_{Dj} - S_{Rj} \quad \text{at } z = 0 \quad (3.3)$$

$$VC_j - y \frac{\partial C_j}{\partial y} = q_{Cj} \text{ or } C_j = C_{oj} \quad \text{at } y = 0 \text{ and } B \quad (3.4)$$

where

B = width of the river of study area

C_{oj} = constant concentration of j^{th} sediment

h = flow depth

q_{Cj} = lateral influx of j^{th} sediment

S_{Dj} = sediment deposition rate per unit bed surface area for j^{th} sediment size fraction

S_{Rj} = sediment erosion rate per unit bed surface area for j^{th} sediment size fraction

γ = coefficient, i.e., probability that particle settling to the bed is deposited.

In this study, γ was assumed to be unity; that is, for the same flow condition all suspended matter settling on the river and ocean beds stays on the beds without returning to the flow. It is also assumed that the vertical flow velocity, W , is negligible.

Let

$$C_j = \bar{C}_j + c_j \quad (3.5)$$

$$U = \bar{U} + u'' \quad (3.6)$$

$$V = \bar{V} + v'' \quad (3.7)$$

$$\frac{\partial c_j''}{\partial x} = \frac{\partial c_j''}{\partial y} = \frac{\partial W_{s_j}}{\partial z} = 0 \quad (3.8)$$

where

$\bar{c}_j, \bar{U}, \bar{V}$ = depth averaged values of concentration of sediment for j^{th} size fraction, longitudinal velocity, and lateral velocity, respectively

c_j'', u'', v'' = fluctuations from the depth averaged values of concentration of sediment of j^{th} size fraction, longitudinal velocity, and lateral velocity, respectively.

By substituting the above expressions into Equation (3.1) and integrating it over the entire river depth, this equation becomes:

$$\begin{aligned}
 \bar{c}_j \left\{ \frac{\partial h}{\partial t} + \frac{\partial}{\partial x}(\bar{U}h) + \frac{\partial}{\partial y}(\bar{V}h) \right\} - (\bar{c}_j + c_j'') \Big|_{z=h} \left\{ \frac{\partial h}{\partial t} + (\bar{U} + u'') \Big|_{z=h} \frac{\partial h}{\partial x} \right. \\
 \left. + (\bar{V} + v'') \Big|_{z=h} \frac{\partial h}{\partial y} \right\} + \left\{ W_{sj} (\bar{c}_j + c_j'') \Big|_{z=h} + \epsilon_z \frac{\partial (\bar{c}_j + c_j'')}{\partial z} \Big|_{z=h} \right\} \\
 = -h \left(\frac{\partial \bar{c}_j}{\partial t} + \bar{U} \frac{\partial \bar{c}_j}{\partial x} + \bar{V} \frac{\partial \bar{c}_j}{\partial y} \right) + h \frac{\partial}{\partial x} \left(\epsilon_x \frac{\partial \bar{c}_j}{\partial x} \right) + h \frac{\partial}{\partial y} \left(\epsilon_y \frac{\partial \bar{c}_j}{\partial y} \right) \\
 - \frac{\partial}{\partial x} \int_0^h u'' c_j'' dz - \frac{\partial}{\partial y} \int_0^h v'' c_j'' dz - \left\{ W_{sj} (\bar{c}_j + c_j'') \Big|_{z=0} \right. \\
 \left. + \epsilon_z \frac{\partial (\bar{c}_j + c_j'')}{\partial z} \Big|_{z=0} \right\} \quad (3.9)
 \end{aligned}$$

The equation of continuity, the kinetic water surface boundary condition and Equation (3.2) make the left side of Equation (3.9) zero. As in the Boussinesq diffusion coefficient concept, let:

$$\int_0^h u'' c_j'' dz = \overline{(u'' c_j'')} h = -h D_x \frac{\partial \bar{c}_j}{\partial x} \quad (3.10)$$

and

$$\int_0^h v'' c_j'' dz = (\overline{v'' c_j''})h = -h D_y \frac{\partial \bar{c}_j}{\partial y} \quad (3.11)$$

where D_x and D_y equal the dispersion coefficients of x and y directions. Hence, Equations (3.2), (3.3), (3.9), (3.10), and (3.11) yield the following final expression of sediment transport:

$$\begin{aligned} \frac{\partial \bar{c}_j}{\partial t} + \left(U - \frac{D_x}{h} \frac{\partial h}{\partial x} \right) \frac{\partial \bar{c}_j}{\partial x} + \left(V - \frac{D_y}{h} \frac{\partial h}{\partial y} \right) \frac{\partial \bar{c}_j}{\partial y} \\ = \frac{\partial}{\partial x} \left(K_x \frac{\partial \bar{c}_j}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y \frac{\partial \bar{c}_j}{\partial y} \right) + \frac{S_{Rj}}{h} - \frac{S_{Dj}}{h} \end{aligned} \quad (3.12)$$

where

$$K_x = \epsilon_x + D_x$$

$$K_y = \epsilon_y + D_y$$

The finite element method was used to solve Equations (3.4) and (3.12). In order to solve Equations (3.4) and (3.12), sediment erosion and deposition rates, S_{Rj} and S_{Dj} , must be evaluated for rivers, estuaries and oceans.

Rivers and Estuaries. Sediment erosion and deposition rates were evaluated separately for each sediment size fraction because erosion and deposition characteristics are significantly different for cohesive and noncohesive sediments.

Erosion and deposition of noncohesive sediments (sand and gravel) are affected by the amount of sediment the flow is capable of carrying. For example, if the amount of sand being transported is less than the flow can carry for given hydrodynamic and wave conditions, the current and waves will scour sediment from the stream bed to increase the sediment transport rate. This occurs until the actual sediment transport rate becomes equal to the carrying capacity of the flow or until the available bed sediments are all scoured, whichever occurs first. Conversely, the flow deposits sand if its

actual sediment transport rate is above the flow's capacity to carry sediment. Because of its simplicity, the following DuBoy's formula was used to calculate the flow capacity of sediment transport, Q_T :

$$Q_T = B \psi_D \tau_b (\tau_b - \tau_c) \quad (3.13)$$

where

B = entire river width or a portion of it

τ_b = bed shear stress

τ_c = critical bed shear stress at which sediment movement begins.

ψ_D = coefficient.

The flow capacity, Q_T , was then compared with the actual amount of sand, Q_{Ta} , being transported in the water. Hence:

$$S_{Rj} = \frac{Q_T - Q_{Ta}}{A} \quad (3.14)$$

$$S_{Dj} = \frac{Q_{Ta} - Q_T}{A} \quad (3.15)$$

where

A = entire river bed surface area or a portion of it.

For sediment erosion and deposition rates of cohesive sediments (silt and clay), the following Partheniades⁽²⁴⁾ and Krone⁽²⁵⁾ formulas were adopted:

$$S_{Rj} = M_j \left(\frac{\tau_b}{\tau_{cRj}} - 1 \right) \quad (3.16)$$

$$S_{Dj} = 2W_{sj}C_j \left(1 - \frac{\tau_b}{\tau_{cDj}} \right) \quad (3.17)$$

where

- M_j = erodibility coefficient for sediment of j^{th} size fraction
 τ_{CD_j} = critical shear stress for sediment deposition for j^{th} sediment size fraction
 τ_{CR_j} = critical shear stress for sediment erosion for j^{th} sediment fraction.

Values of M_j , τ_{CD_j} and τ_{CR_j} must be determined by field and/or laboratory tests. These values for the Columbia River (Washington) and the Clinch River (Tennessee) were reported in recent mathematical simulation studies concerning sediment and radionuclide transport in these two rivers.^(5,26) The availability of bed sediments to be resuspended was also examined to determine the actual amount of sediment erosion.

When the fall velocity, W_{sj} , depends on sediment concentration and no aggregation occurs, the fall velocity may be assumed:⁽²⁵⁾

$$W_{sj} = K_j' C_j^{4/3} \quad (3.18)$$

where

K_j' = an empirical constant depending on the sediment type.

Oceans and the Great Lakes with surface waves. When surface waves are present, it is assumed that wave motion is a dominant mechanism for suspension of sediment which will then be transported by a combination of an ambient velocity of incidental flow (other than that included by wave motion) and the second order velocity components of waves. In this case, the DuBoy's formula for calculating transport of noncohesive sediment in rivers and estuaries was replaced by appropriate wave-sediment transport formulas, as will be discussed below. Because of the lack of formulations to calculate rates of the cohesive sediment erosion and deposition by waves, Partheniades and Krone's formulas (Equations 3.16 and 3.17) for cohesive sediment (silt and clay) were also used for marine environment.

Off shore zone: With the wave energy spectrum as a starting point, some results of various researchers^(27,28) were used to obtain the wave induced sediment suspension in offshore zones. Both the wave-induced bed load and suspended sediment concentrations were calculated. For the bed load concentrations the approach was based upon the following argument:⁽²⁷⁾ the probability that a sediment particle is set into motion is the same as the probability that the instantaneous lift on the particle is greater than its submerged weight. This probability, denoted by p , is given as follows:

$$p = \frac{1}{\sqrt{2\pi}} \int_{B^*\psi - 1/\zeta_0}^{\infty} e^{-z^2/2} dz \quad (3.19)$$

where

$$\psi = \frac{(\rho_s - \rho)}{\rho \bar{u}^2} gD$$

$$B^* = 4$$

$$1/\zeta_0 = 1.5$$

$$\rho_s = \text{sediment density}$$

$$\rho = \text{water density}$$

$$\gamma_s = \text{unit weight of sediment}$$

$$g = \text{gravitational acceleration}$$

$$D = \text{equivalent sediment particle diameter}$$

$$\bar{u} = \text{average horizontal velocity in the boundary layer.}$$

The bed load concentration, C_o , is given by the relation equation

$$\bar{C}_o = A_o p \gamma_s \quad (3.20)$$

where A_o is a constant which must be determined by experiment. Thus, with a known A_o value, C_o can be calculated if u is known (see the expression for ψ).

The velocity $\bar{u}$ is obtained by treating the flow field in the turbulent boundary layer as a superposition of all the components in the random wave train. Thus, $\bar{u}^2$ can be written as:

$$\bar{u}^2 = \sum_i (u_{oi}^2) (1 - 2 f_{1i} \cos f_{2i} + f_{1i}^2) \quad (3.21)$$

where

$$f_{1i} = 0.5 \exp \frac{[-133 \sinh (k_i h) y]}{a_i \beta_i D}$$

$$f_{2i} = 0.3 (\beta_i y)$$

$$\beta_i = \frac{\omega_i}{2\nu}$$

a_i = wave amplitude

ω_i = wave frequency (rad/sec)

h = water depth

k_i = wave number

y = vertical coordinate

$u_{oi} = a_i \omega_i / \sinh (\beta_i h)$

ν = kinematic viscosity of water.

The average bed load transport Q_B is obtained by integrating as follows:

$$Q_B = \bar{C}_o \int_0^{2D} (U_B + U_{AB}) dz \quad (3.22)$$

where

U_{AB} = velocity component of incidental flow (other than that induced by a wave action) near the ocean bed

U_B = mass transport velocity (second order velocity components) of a wave near the ocean bed.

U_B is calculated by expression obtained by Liang and Wang.⁽²⁷⁾ The distribution of vertical velocity of the incidental flow is assumed to follow the 1/7-th-power law.⁽²⁹⁾ Hence, the bed load is transported by both wave induced velocity and the incidental flow.

The concentration of the suspended sediment is calculated by taking the time average of the diffusion equation and solving a resulting linear elliptic equation obtained by neglecting the molecular diffusion coefficient and estimating the diffusion coefficients of wave motion and turbulence. The suspended sediment concentration at elevation z with no depth restriction is given by:⁽²⁷⁾

$$\frac{C}{C_0} = \left[\frac{\tanh(kz/2)}{\tanh(kz_0/2)} \right] R_i, \quad z_0 = 2D \quad (3.23)$$

$$R_i = \frac{W_s \sinh k_i h}{\gamma \sigma k_i a_i \omega_i} \quad (3.24)$$

where

ω_i = frequency

h = water depth

k_i = wave number

$\gamma = 3/(2 \rho_s/\rho + 1)$

σ = constant

a_i = wave amplitude

W_s = sediment settling velocity

z = vertical coordinate.

For the case of shallow water, the suspended sediment concentration C at the elevation z is given by:⁽²⁷⁾

$$\frac{C}{C_0} = \left(\frac{2D}{z} \right) |R_i| \quad (3.25)$$

$$R_i = \frac{W_s h}{\gamma \sigma a_i \omega_i} \quad (3.26)$$

For this study, Equations (3.25) and (3.26) for a shallow water case were used. The rate of suspended sediment transport in the interior zone (Q_S) was then obtained as:

$$Q_S = \int_{2D}^h C (U_S + U_{IS}) dz \quad (3.27)$$

where

U_{IS} = velocity component of incidental flow (other than that induced by wave action) in the interior zone)

U_S = mass transport velocity (second order velocity component) of a wave in the interior zone.

The mass transport velocity U_S is calculated by Liang and Wang's expression.⁽²⁷⁾ The vertical velocity distribution of the incidental flow is assumed to follow the 1/7-th-power law. Hence, suspended sediment is also transported by both wave-induced velocity and the incidental flow.

Hence, the transport capacity of flow for noncohesive sediment, Q_T , is:

$$Q_T = Q_B + Q_S \quad (3.28)$$

Q_T , thus obtained, can then be used to calculate the erosion and/or deposition rates of sand by Equations (3.13) and (3.14).

Surf zone: The formulations discussed above are only applicable to regions well beyond the surf zone. The following expressions were used in the FETRA code to include the littoral (longshore) transport of sediments in the surf zone induced by the energy and momentum expended by breaking waves. The work of Komar⁽³⁰⁾ and some of his associates was adopted for this study. The volumetric littoral transport rate S_ℓ and the immersed weight littoral transport rate I_ℓ are given by:⁽³⁰⁾

$$S_\ell = \frac{I_\ell}{(\rho_s - \rho) g a^3} \quad (3.29)$$

$$I_\ell = 0.28 (ECn)_b \frac{\bar{v}_\ell}{u_m} \quad (3.30)$$

$$u_m = \left[\frac{2E_b}{\rho h_b} \right]^{1/2} \quad (3.31)$$

where

$(EC_n)_b$ = the energy flux of the waves evaluated at the breaker zone

E_b = the energy of the breaking waves

h_b = the water depth at breaking

$\bar{v}_\ell$ = velocity caused by the combination of waves and currents,

$$(\bar{v}_\ell = 2.7 U_m \sin \alpha_b \cos \alpha_b + U_I)$$

α_b = breaker angle with the shoreline

U_I = velocity of incidental flow (other than that induced by waves) in a surf zone, and

a' = an empirical constant (≈ 0.6).

In the case where the mass transport is induced by wave action alone (in the absence of other currents, i.e., $U_I = 0$), the longshore velocity becomes:

$$\bar{v}_\ell = 2.7 U_m \sin \alpha_b \cos \alpha_b \quad (3.32)$$

Hence, the transport rates for this case are given by

$$S_\ell = (6.85 \times 10^{-5}) (EC_n)_b \sin \alpha_b \cos \alpha_b \quad (3.33)$$

$$I_\ell = 0.77 (EC_n)_b \sin \alpha_b \cos \alpha_b \quad (3.34)$$

Therefore, the total sediment transport capacity, Q_T , is then calculated by:

$$Q_T = a \cdot S_\ell \quad (3.35)$$

where a = unit conversion constant.

Rates of erosion and deposition of noncohesive sediment in a surf zone are then calculated by Equations (3.14) and (3.15).

In order to use the above formulas for the littoral transport of sediment bound radionuclides, the wave angle at breaking α_b must be calculated. This was accomplished with the wave refraction program which was used in conjunction with FETRA. This program was developed by Dobson,⁽³¹⁾ and later modified by Ecker and Degraça.⁽³²⁾ The theoretical basis of the wave refraction program is derived from geometrical optics and utilizes Snell's Law. The program utilizes wave hindcast data to obtain the representative deepwater waves for all wave directions and periods. From these deepwater

waves, the program simulates the process by which each appropriate deepwater wave ray is generated towards shore. Starting from a known point on a contour grid with a given period and an initial direction, the computer program constructs a single wave ray step by step across the grid. At breaking, the program calculates the refraction coefficient, K_R , shoaling coefficient, K_S , the wave angle at breaking, α_b , the depth at breaking, d_b , and the wave height, h_b . The program also computes the alongshore component of wave power at designated stations along the shoreline. As discussed above, it is assumed that rates of erosion and deposition of cohesive sediments in oceans and the Great Lakes are also expressed by Equations (3.16) and (3.17).

Dissolved Contaminant Transport Model

The association of dissolved contaminants (such as radionuclides, heavy metals, pesticides and nutrients) with suspended sediments is assumed to be the primary mechanism of contaminant uptake. Consequently, the model includes the effects of:

1. convection and dispersion of dissolved contaminant
2. adsorption (uptake) of dissolved contaminant by sediments (cohesive and noncohesive sediments) or desorption from the sediments into water
3. chemical and biological decay of contaminant
4. contaminant contributions from tributaries (contaminant contributions from wastewater discharges, overland runoff flow, fallout and ground water to a surface water system may be treated as a part of tributary contributions).

Effects of water quality (e.g., pH, water temperature, salinity, etc.) and sediment characteristics (e.g., clay minerals) are taken into account through changes in the distribution (or partition) coefficient, K_{d_j} , and transfer rate, K_j .

The governing equation of dissolved contaminant transport for the three-dimensional case is:

$$\frac{\partial G_w}{\partial t} + \frac{\partial}{\partial x} (UG_w) + \frac{\partial}{\partial y} (VG_w) + \frac{\partial}{\partial z} (WG_w)$$

$$\begin{aligned}
&= \frac{\partial}{\partial x} (\epsilon_x \frac{\partial G_w}{\partial x}) + \frac{\partial}{\partial y} (\epsilon_y \frac{\partial G_w}{\partial y}) + \frac{\partial}{\partial z} (\epsilon_z \frac{\partial G_w}{\partial z}) \\
&- \lambda G_w - \sum_j K_j (K_{dj} C_j G_w - C_j G_j)
\end{aligned} \tag{3.36}$$

In addition to the previously defined symbols:

K_{dj} = distribution (or partition) coefficient between dissolved contaminant and particulate contaminant associated with j^{th} sediment

K_j = transfer rate of contaminant for j^{th} sediment

G_j = particulate contaminant concentration associated with j^{th} sediment (weight or contaminant per unit weight of sediment)

G_w = dissolved contaminant concentration (weight of contaminant per unit volume of water)

λ = chemical and biological decay rates of contaminant

Distribution coefficient, K_{dj} , is defined by:

$$K_{dj} = \frac{f_{sj} / M_j'}{f_w / V_w} = \frac{f_{sj}}{f_w C_j} \tag{3.37}$$

where

f_{sj} = fraction of contaminant sorbed by j^{th} sediment

f_w = fraction of contaminant left in solution

M_j' = weight of j^{th} sediment

V_w = volume of water

$$\frac{f_{sj}}{f_w} = \frac{C_j G_j}{G_w}$$

Hence Equation (3.37) may be rewritten as:

$$G_j = K_{dj} G_w \tag{3.38}$$

The adsorption of contaminant by sediments or desorption from the sediments is assumed to occur toward an equilibrium condition with the transfer rate, K_j , if the particulate contaminant concentration differs from its equilibrium values as expressed in Equation (3.38).

The boundary conditions for dissolved pollutant transport are:

$$WG_w - \epsilon_z \frac{\partial G_w}{\partial z} = 0 \quad \text{at } z = h \quad (3.39)$$

$$\frac{\partial G_w}{\partial z} = 0 \quad \text{at } z = 0 \quad (3.40)$$

$$VG_w - \epsilon_y \frac{\partial G_w}{\partial y} = q_w \text{ or } G_w = G_{w0} \quad \text{at } y = 0 \text{ and } B \quad (3.41)$$

Let:

$$G_w = \bar{G}_w + G_w'' \quad (3.42)$$

$$\frac{\partial G_w''}{\partial x} = \frac{\partial G_w''}{\partial y} = 0 \quad (3.43)$$

where

G_w'' = fluctuation from the depth averaged value of pollutant concentration

G_{w0} = constant concentration of dissolved contaminant

q_w = lateral influx of dissolved contaminant

By substituting the above expressions with those in Equations (3.5) through (3.8), into Equation (3.36) and integrating it over the entire river depth, Equation (3.36) becomes:

$$\begin{aligned} \bar{G}_w \left\{ \frac{\partial h}{\partial t} + \frac{\partial}{\partial x} (\bar{U}h) + \frac{\partial}{\partial y} (\bar{V}h) \right\} - (\bar{G}_w + G_w'') \bigg|_{z=h} \left\{ \frac{\partial h}{\partial t} + (\bar{U} + u'') \bigg|_{z=h} \frac{\partial h}{\partial x} \right. \\ \left. + (\bar{V} + v'') \bigg|_{z=h} \frac{\partial h}{\partial y} \right\} + \left\{ (\bar{W} + w'') (\bar{G}_w + G_w'') \bigg|_{z=h} - \epsilon_z \frac{\partial}{\partial z} (\bar{G}_w + G_w'') \bigg|_{z=h} \right\} \end{aligned}$$

$$\begin{aligned}
& + \epsilon_z \frac{\partial}{\partial z} (\bar{G}_w + G_w'') \Big|_{z=0} \\
& = -h \left(\frac{\partial \bar{G}_w}{\partial t} + \bar{U} \frac{\partial \bar{G}_w}{\partial x} + \bar{V} \frac{\partial \bar{G}_w}{\partial y} + D_x \frac{\partial h}{\partial x} \frac{\partial \bar{G}_w}{\partial x} + D_y \frac{\partial h}{\partial y} \frac{\partial \bar{G}_w}{\partial y} \right. \\
& + h \frac{\partial}{\partial x} \left\{ (\epsilon_x + D_x) \frac{\partial \bar{G}_w}{\partial x} \right\} + h \frac{\partial}{\partial y} \left\{ (\epsilon_y + D_y) \frac{\partial \bar{G}_w}{\partial y} \right\} \\
& \left. - \lambda h \bar{G}_w - h \sum_j K_j \bar{C}_j (K_{d_j} \bar{G}_w - K_{p_j} G_j) \right\} \quad (3.44)
\end{aligned}$$

The equation of continuity, the kinetic water surface boundary condition and boundary conditions shown in Equations (3.39) and (3.40) then make the left side of Equation (3.44) zero. Hence, the final transport equation of dissolved pollutant is:

$$\begin{aligned}
& \frac{\partial \bar{G}_w}{\partial t} + \left(\bar{U} - \frac{D_x}{h} \frac{\partial h}{\partial x} \right) \frac{\partial \bar{G}_w}{\partial x} + \left(\bar{V} - \frac{D_y}{h} \frac{\partial h}{\partial y} \right) \frac{\partial \bar{G}_w}{\partial y} \\
& = \frac{\partial}{\partial x} \left(k_x \frac{\partial \bar{G}_w}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \frac{\partial \bar{G}_w}{\partial y} \right) - (\lambda + \sum_j K_j K_{d_j} \bar{C}_j) \bar{G}_w \\
& + \sum_j K_j \bar{C}_j G_j \quad (3.45)
\end{aligned}$$

The boundary conditions for this equation are those in Equation (3.41).

Particulate Contaminant Transport Model

The transport model of contaminants attached to sediments is solved separately for those adsorbed by cohesive and noncohesive sediments. This model also includes the effects of:

1. convection and dispersion of particulate contaminant
2. adsorption (uptake) of dissolved contaminant by sediments or desorption from sediments into water

3. chemical and biological decay of contaminant
4. deposition of particulate contaminant on the river and ocean beds or resuspension from the beds
5. contaminant contributions from tributaries (again, contaminant contributions from wastewater discharges, overland runoff flow, fallout and ground water to a surface water system may be treated as a part of the tributary contributions).

As in the transport of sediments and dissolved contaminant, the three-dimensional transport equation for contaminants adsorbed by the j^{th} sediment size may be expressed as:

$$\begin{aligned} \frac{\partial C_j G_j}{\partial t} + \frac{\partial}{\partial x}(U C_j G_j) + \frac{\partial}{\partial y}(V C_j G_j) + \frac{\partial}{\partial z} \left\{ (W - W_{s_j}) C_j G_j \right\} &= \frac{\partial}{\partial x} \left(\epsilon_x \frac{\partial C_j G_j}{\partial x} \right) \\ &+ \frac{\partial}{\partial y} \left(\epsilon_y \frac{\partial C_j G_j}{\partial y} \right) + \frac{\partial}{\partial z} \left(\epsilon_z \frac{\partial C_j G_j}{\partial z} \right) - \lambda C_j G_j - K_j (C_j G_j \\ &- K_{d_j} C_j G_w) \end{aligned} \quad (3.46)$$

where the particulate contaminant concentration, G_j , is assumed to be independent of z .^(5,26) All symbols in Equation (3.46) were previously defined. Noting Equations (3.2), (3.3), and (3.4), the boundary conditions for this case become:

$$(W - W_{s_j}) G_j G_j - \epsilon_z \frac{\partial C_j G_j}{\partial z} = G_j \left\{ (W - W_{s_j}) C_j - \epsilon_z \frac{\partial C_j}{\partial z} \right\} = 0 \quad \text{at } z = h \quad (3.47)$$

$$(1 - \gamma) W_{s_j} C_j G_j + \epsilon_z \frac{\partial C_j G_j}{\partial z} = G_j S_{D_j} - G_{B_j} S_{R_j} \quad \text{at } z = 0 \quad (3.48)$$

$$V C_j G_j - \epsilon_y \frac{\partial C_j G_j}{\partial y} = q_j \quad \text{or } G_j = G_{Oj} \quad \text{at } y = 0 \text{ and } B \quad (3.49)$$

where

G_{B_j} = a particulate contaminant concentration associated with j^{th} sediment in river (or ocean) bed.

G_{oj} = constant concentration of particulate contaminant associated with j^{th} sediment

q_j = lateral influx of particulate concentration associated with j^{th} sediment

Equation (3.50) is derived by 1) substituting Equations (3.5) through (3.8) into Equation (3.46), 2) integrating it over the river depth, 3) then substrating equation Equation (3.9) multiplied by G_j from the resulting equation, and 4) substituting the boundary conditions, Equations (3.47) and (3.48):

$$\begin{aligned} \frac{\partial G_j}{\partial t} + \left\{ \bar{U} - \frac{2\epsilon_x}{C_j} \frac{\partial \bar{C}_j}{\partial x} - \frac{D_{xj}}{C_j} \frac{\partial \bar{C}_j}{\partial x} + \frac{\epsilon_x}{C_{jh}} \frac{\partial h}{\partial x} c_{jz}'' \Big|_z=h \right\} \frac{\partial G_j}{\partial x} \\ + \left\{ \bar{V} - \frac{2\epsilon_y}{C_j} \frac{\partial \bar{C}_j}{\partial y} - \frac{D_{yj}}{C_j} \frac{\partial \bar{C}_j}{\partial y} + \frac{\epsilon_y}{C_{jh}} \frac{\partial h}{\partial y} c_{jz}'' \Big|_z=h \right\} \frac{\partial G_j}{\partial y} \\ = \frac{\partial}{\partial x} \left(\epsilon_x \frac{\partial G_j}{\partial x} \right) + \frac{\partial}{\partial y} \left(\epsilon_y \frac{\partial G_j}{\partial y} \right) - \left(\frac{S_{Rj}}{C_{jh}} + \lambda + K_j G_j \right) \\ + \left(K_j K_{dj} G_w + \frac{G_{Bj} S_{Rj}}{C_{jh}} \right) \end{aligned} \quad (3.50)$$

Since the two terms containing "c" in the above equation are at least one order of magnitude smaller than the rest of the terms, these two terms may be omitted. Hence, the final expression becomes:

$$\begin{aligned} \frac{\partial G_j}{\partial t} + \left\{ \bar{U} - \frac{2\epsilon_x}{C_j} \frac{\partial \bar{C}_j}{\partial x} - \frac{D_{xj}}{C_j} \frac{\partial \bar{C}_j}{\partial x} \right\} \frac{\partial G_j}{\partial x} + \left\{ \bar{V} - \frac{2\epsilon_y}{C_j} \frac{\partial \bar{C}_j}{\partial y} - \frac{D_{yj}}{C_j} \frac{\partial \bar{C}_j}{\partial y} \right\} \frac{\partial G_j}{\partial y} \\ = \frac{\partial}{\partial x} \left(\epsilon_x \frac{\partial G_j}{\partial x} \right) + \frac{\partial}{\partial y} \left(\epsilon_y \frac{\partial G_j}{\partial y} \right) - \left(\frac{S_{Rj}}{C_{jh}} + \lambda + K_j G_j \right) \\ + \left(K_j K_{dj} G_w + \frac{G_{Bj} S_{Rj}}{C_{jh}} \right) \end{aligned} \quad (3.51)$$

The boundary conditions for this case are those expressed in Equation (3.49).

Finite Element Method

Because of its increased solution accuracy and ready accommodation to various boundary geometrics, the finite element method was selected for this study. The finite element solution technique with the Galerkin weighted residual method is used to solve Equations (3.12), (3.45) and (3.51) with the boundary conditions of Equations (3.4), (3.41) and (3.49).

The flow domain is divided into a series of triangular elements interconnected at node points. Six nodes are associated with each triangle, three at the vertices called corner nodes and three on the mid-sides called mid-side nodes. A quadratic approximation is made for the sediment and contaminant concentrations within each element. Either linear or quadratic interpolation is used for the variation of flow depth and velocity within an element.

The computer program was written in FORTRAN IV language to implement the model for a CDC 7600 computer.

Data Requirements of FETRA

All of the input data required to operate FETRA are listed below for each submodel of FETRA:

All submodels:

- Channel geometry or bathymetry
- Depth and velocity distributions which will be obtained by the hydrodynamic code RMA II with field data
- Longitudinal and lateral dispersion coefficients.

Sediment transport model:

- Sediment size distribution
- Sediment density and fall velocity
- Critical shear stresses of erosion and deposition of cohesive sediments (silt and clay)

- Erodibility coefficient for erosion of cohesive sediment
- For marine environments wave characteristics of deep water

Wave number

Wave height

Wave frequency

Direction of wave propagation

These wave characteristics are used to calculate wave angles in a study area by the Wave Refraction model. Computed wave angles in the study area will then be used for FETRA to simulate sediment-wave interaction.

- Initial conditions

Sediment concentrations for each sediment size fraction

Bottom sediment size fraction

- Boundary conditions

Sediment concentration or its gradient at the boundaries

Dissolved and particulate contaminant transport submodels:

- Distribution coefficients of contaminants with river and marine sediments for each sediment size fraction

- Initial conditions

Dissolved contaminant concentration

Particulate contaminant concentration associated with sediment in water for each sediment size fraction

Particulate contaminant concentration for each sediment size fraction within river and ocean beds

- Boundary conditions

Dissolved contaminant concentration or its gradient at the boundaries

Particulate contaminant concentration or its gradient at the boundaries for each sediment size fraction.

Concentrations of sediments and particulate radionuclide associated with each sediment size fraction as initial and boundary conditions are desirable. However, if these detailed data are not available, they may be estimated by concentrations of bulk sediment and particulate contaminant concentrations attached to bulk sediment, with the sediment size distribution and clay mineral.

Output of FETRA

The FETRA code then computes the following:

Sediment simulation for any given time:

- longitudinal and lateral distributions of total sediment (sum of suspended and bed load) concentration for each sediment size fraction
- three-dimensional (longitudinal, lateral and vertical) distributions of ratio of different sediment size fraction in the river and ocean beds
- change in bed elevation (elevation changes due to sediment deposition and/or scour)

Contaminant simulation for any given time:

- longitudinal and lateral distributions of dissolved contaminant concentration
- longitudinal and lateral distributions of contaminant concentration adsorbed by sediment for each sediment size fraction
- three-dimensional distributions of contaminant concentrations in the bottom sediment within the bed for each sediment size fraction.

Modeling Procedure

The modeling procedure of radionuclide migration in rivers, estuaries, oceans and the Great Lakes is shown in Figure 1. The sequence of modeling is shown by the direction of the arrows. As indicated in this figure, the procedure consists of the following three steps:

1. "Field Data Collection" to supply necessary input data to various mathematical models.
2. "Mathematical Modeling" consisting of the following substeps to simulate river flows, tidal flows, ocean currents, waves and transport of sediment and contaminants.
 - 2.1 "Hydrodynamic Modeling by RMA II" to obtain velocity and depth distributions
 - 2.2 "Wave Dynamic Modeling by Wave Refraction Model" to predict temporal and spatial distributions of wave angles for marine environments.
 - 2.3 "Sediment and Contaminant Transport by FETRA" which consists of the following four steps performed by the model, FETRA, internally,
 - 2.3.1 "Sediment Transport Modeling" involving sediment transport simulation.
 - 2.3.2 "Dissolved Contaminant Transport Modeling" to simulate dissolved contaminant movement by including the interaction with sediments.
 - 2.3.3 "Particulate Contaminant Transport Modeling" to simulate particulate contaminant movements by including the interaction with dissolved contaminant and sediments.
 - 2.3.4 "River and Ocean Bed Modeling" to simulate changes in river and ocean bed conditions including: 1) river and ocean bed elevation change, 2) distribution of ratio of each bed sediment size fraction in the bed, and 3) distribution of contaminants within the bed.
3. "Analysis of Computer Results" to assess migration of contaminants.

FIGURE 1. Modeling Procedure

4. CURRENT STATUS OF THE STUDY

Literature survey on sediment and contaminant transport modeling in rivers, estuaries, oceans and impoundments, and radionuclide sorption mechanism has been completed. The draft report on this subject was submitted to NRC in May 1978. The final report of this literature survey will be submitted to NRC in early 1979. This report is entitled "Critical Review: Radionuclide Transport, Sediment Transport and Water Quality Mathematical Modeling and Radionuclide Sorption/Desorption Mechanisms," NUREG-CR-0657/PNL-2901, by Y. Onishi, R. J. Serne, E. M. Arnold, C. E. Cowan, F. L. Thompson and R. M. Ecker. The study reveals that models developed by Gloyne and his associates, Field (CHNSED code) and Onishi et al. (SERATRA and FETRA codes) are the only models presently available to simulate both migration of dissolved and particulate radionuclides by sediment-radionuclide interactions for rivers. For oceans and estuaries, only the model FETRA is applicable to simulate migration of both dissolved and particulate contaminants.

Under this study, FETRA, which was originally developed for rivers was modified to be applicable to oceans and the Great Lakes by including wave motion to suspend marine sediments. This modification to FETRA is almost completed; consequently FETRA can now be applied for solving unsteady, two-dimensional distributions of sediment, dissolved and particulate contaminants in rivers, oceans and the Great Lakes. Tests are currently underway on a portion of FETRA which computes suspended and bed sediment load caused by wave actions in offshore and surf zones. A topical report for the mathematical model of sediment and contaminant transport in marine environments is under preparation.

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