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NRC Research and Technical
Assistance Report

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QUARTERLY REPORT
OCTOBER 1979 to DECEMBER 1979

MATHEMATICAL SIMULATION OF SEDIMENT AND CONTAMINANT TRANSPORT IN SURFACE WATERS

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Prepared for the
U.S. Nuclear Regulatory Commission

by
Pacific Northwest Laboratory
Richland, Washington 99352

NRC Research and Technical
Assistance Report

MATHEMATICAL SIMULATION OF SEDIMENT AND CONTAMINANT TRANSPORT IN SURFACE WATERS

OCTOBER 1979 TO DECEMBER 1979

SUMMARY

During the first quarter of FY-1980, we have worked on two tasks: Task B, Transport of Sediment and Radionuclides in Oceans; and Task C, Transport of Sediment and Radionuclides in Estuaries.

Under Task B, FETRA was further tested for 1) its basic computational scheme, and 2) wave-sediment computation scheme by computing sediment transport rate resulting from wave actions under some simple conditions. In addition, flow, sediment and radionuclide data for various coastal sites were collected through a literature search and examined to determine which site should be selected for the FETRA ocean application. Based on a review meeting of this project held on November 16, 1979 at the NRC Headquarters, the Irish Sea was selected for the FETRA ocean modeling site because it appears to have the best data base. Collection of the data required to apply FETRA to the Irish Sea is underway.

Under Task C, work is continuing on the synthesis of three-dimensional model for sediment-radionuclide transport. The model can also calculate hydrodynamics and salinity transport. The model has been tested by comparing predicted three-dimensional flow movements in a hypothetical water body with those predicted by a quasi-three dimensional model developed by Leendertse (Leendertse et al. 1973). The comparison showed good agreement between the two models. Field data collected for various estuaries have been obtained through a literature review to determine an estuarine modeling site.

TASK B: TRANSPORT OF SEDIMENT AND RADIONUCLIDES IN OCEANS

For this task, we are using the sediment-contaminant transport model, FETRA, which is an unsteady, two-dimensional finite element model. FETRA consists of three submodels coupled to include the mechanisms of sediment/contaminant interactions on contaminant transport. The submodels are: 1) a sediment transport submodel, 2) a dissolved contaminant transport submodel, and 3) a particulate contaminant (those adsorbed by sediment) transport submodel.

During FY-1979, the following modifications to FETRA were made (Onishi et al. 1979):

1. to the numerical scheme -
    - linear and quadratic approximations to depth and velocity distributions within each computational finite element cell to improve the compatibility of FETRA with hydrodynamic codes
    - capacity to vary the computational scheme from fully explicit to fully implicit
2. to the sediment submodel -
    - capacity to generate wind-induced wave characteristics
    - inclusion of sediment suspension mechanisms by wave motions in off-shore and surf zones.
3. to the dissolved contaminant submodel -
    - direct radionuclide adsorption/desorption between dissolved radionuclides and non-moving bed sediment
4. to the particulate contaminant submodel -
    - no change
5. to the bed history computation -
    - direct radionuclide adsorption/desorption between dissolved radionuclides and non-moving bed sediment

Some simple testing of the modified version of FETRA was conducted in FY-1979 and the first quarter of FY-1980. The basic computational scheme and the stability criteria of FETRA was tested by comparing its numerical solution with the analytical solution of the following unsteady, advection-diffusion equation:

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial X} = E_x \frac{\partial^2 C}{\partial X^2}$$

Initial Condition:

$$C(X,0) = EXP(\frac{-UX}{2E_X})SIN(\frac{\pi X}{\ell})$$

Boundary Conditions:

$C(0,t) = 0.,\qquad C(\ell,t) = 0$

$U = 2., E_x = 1.$ and $\ell = 1.$

As shown in Figure 1, comparison between computed results and analytical solution indicates good agreement. Stability criteria for FETRA were examined by using this example. The Courant Numbers, CN and diffusion number, D as defined below were used for the stability criteria (Roache 1972);

$$CN = \frac{U\Delta t}{\Delta X}$$

$$D = \frac{Ex\Delta t}{\Delta X^2}$$

Several computer runs were made to indicate the following results at time plane t = 0.2 (see Figure 1 and Table 1).

Equation Solved:

$$\frac{\partial C}{\partial t} + U \frac{\partial C}{\partial X} = E_x \frac{\partial^2 C}{\partial X^2}$$

Initial Condition:

$$C(X,0)=EXP(-\frac{UX}{2E_x})SIN(\frac{\pi X}{\ell})$$

Boundary Conditions:

$C(0,t) = 0.$, ; $C(\ell,t) = 0$

$U = -2.$, $E_x = 1.$ and $\ell = 1.$

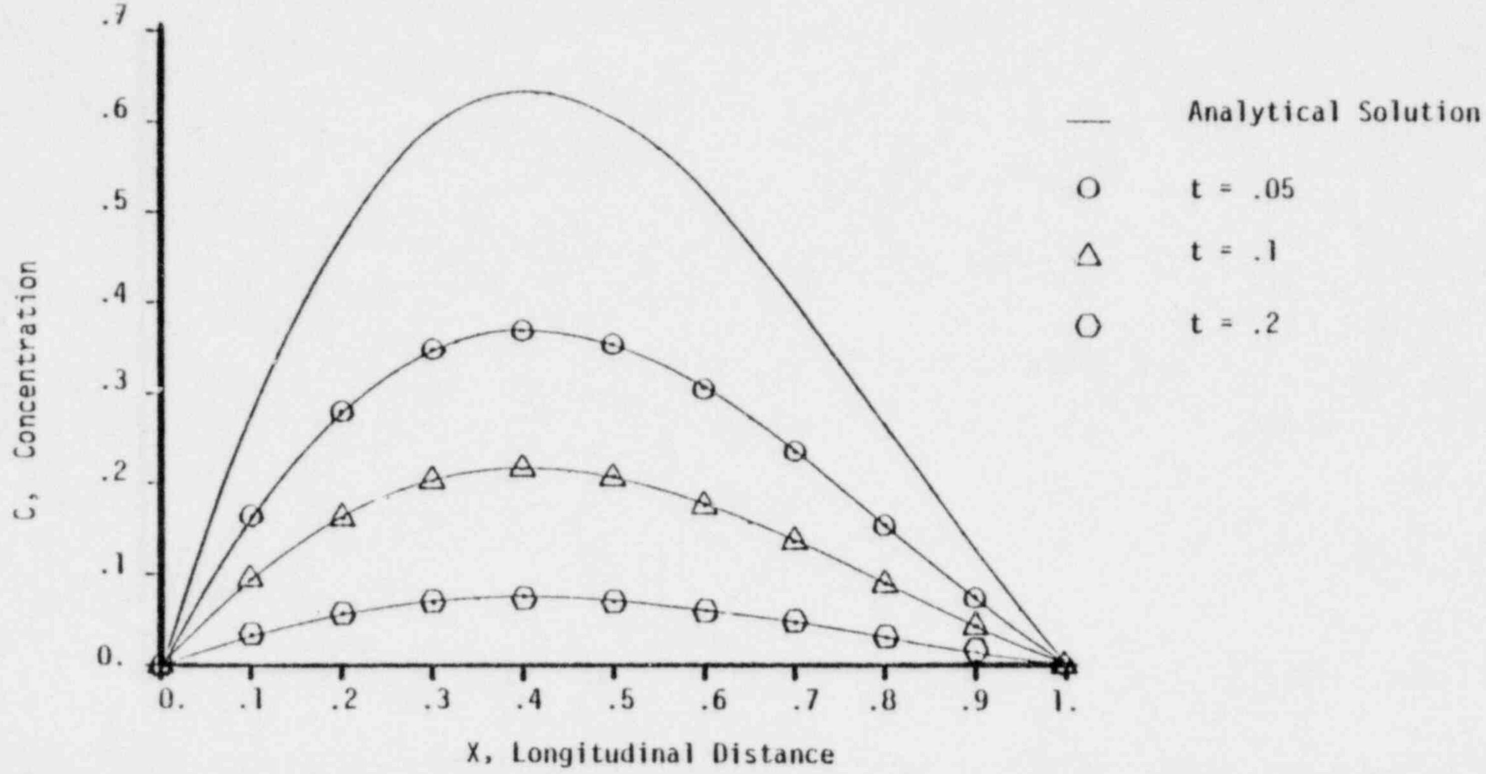

FIGURE 1. Comparison of FETRA and Analytical Solutions to the Unsteady Convection-Diffusion Equation.

TABLE 1. Stability Criteria

Case Number	Stability Criteria: Courant Number CN	Stability Criteria: Diffusion Number, D	Number of Time Steps	Maximum Error in Solutions %
1	0.1	0.5	40	-0.16
2	0.5	2.5	8	-1.5
3	1.0	5.0	4	-5.9

These results indicate that, under the conditions tested, combinations of Courant and Diffusion Numbers of 0.5 and 2.5 may be used if errors in solutions can be allowed several percent. However, if a long term simulation is derived (that is if a number of time steps is large), then CN and D values may have to be reduced to say 0.1 and 0.5, respectively.

Simple examples of calculated noncohesive sediment load due to wind-induced waves in an offshore zone are shown in Table 2 and Figure 2. Table 2 indicates six different wind conditions (25 knots to 50 knots) tested to generate surface waves which, in turn, suspend marine sediment. It was assumed that there are no external flow components except those caused by wave actions alone.

TABLE 2. Test Conditions of Sand Transport Capacities

Case	Wind Velocity, knots	Flow Depth, in.	Fetch Length, km
1	25	7.5	80
2	30	7.5	80
3	35	7.5	80
4	40	7.5	80
5	45	7.5	80
6	50	7.5	80

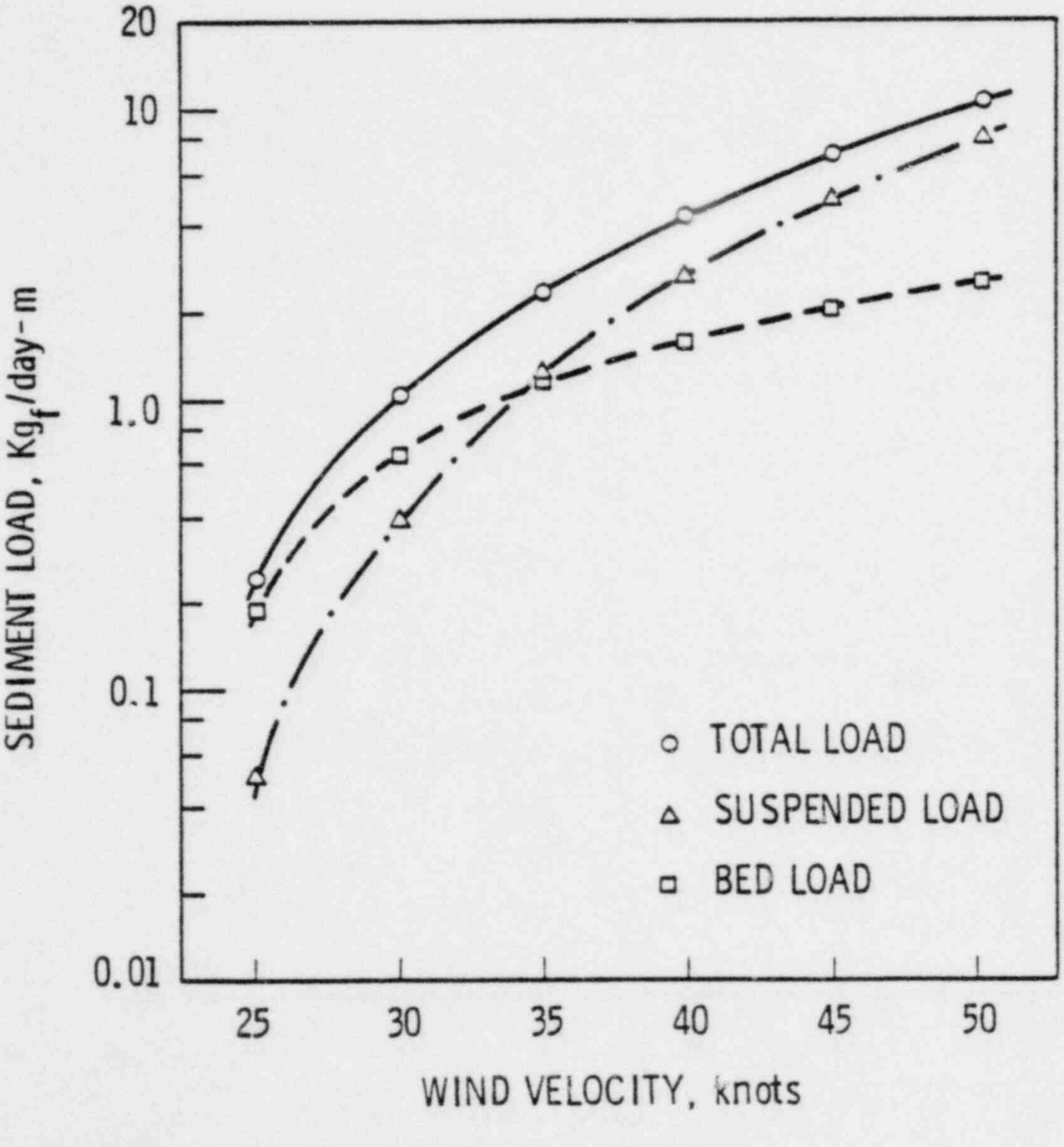

FIGURE 2. Calculated Sediment Load Due to Wind-Induced Wave in Marine Environment

Computed suspended, bed and total (sum of suspended and bed loads) load are shown in Figure 2. The computed sediment load (both suspended and bed sediment loads) increases with wind velocity and increments of suspended load is greater than those of bed load as wind velocity increases, as expected. For example, at the wind speed of 25 knots, bed load consists of 80% of the total load, whereas the suspended load is only 20% of the total. However, at the wind speed of 50 knot, bed load is only 25% of the total and suspended load consists of 75%. However, there are no measured data to check the computed results.

The next step is to verify the FETRA model 1) by applying the model to a coastal water to simulate migration of sediment and radionuclides and 2) by comparing computed results with field data. 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 a hydrodynamic code (e.g., CAFE) with field data
- Longitudinal and lateral dispersion coefficients.

Sediment transport submodel:

- Sediment size distribution and density
- Sediment fall velocity (it can be estimated by sediment sizes and density)
- Critical shear stresses of erosion and deposition of cohesive sediments (silt and clay) (they are usually selected through a model calibration process)
- Erodability coefficient for erosion of cohesive sediment (it is usually selected through a model calbiration process)
- For marine environments

  a) Wave characteristics of deep water

Wave number Wave height Wave frequency Direction of wave propagation	They are used to calculate wave characteristics in a study area (in off-shore and surf zones) by the Wave Refraction Model (Dobson 1967, and Degraca 1974)

or

b) Information to generate wind-induced waves
   Wind velocity
   Mean fetch depth
   Effective fetch length

- Initial conditions
  - Sediment concentrations for each sediment size fraction
  - Bottom sediment size fraction
- Boundary conditions
  - Concentration or lateral influx of sediment at the boundaries

Dissolved and particulate contaminant (radionuclide) transport submodels:

- Distribution coefficients of radionuclide with marine sediments for each sediment size fraction
- Initial conditions
  - Dissolved radionuclide concentration
  - Particulate radionuclide concentration associated with sediment in water for each sediment size fraction
  - Particulate radionuclide concentration for each sediment size fraction within ocean bed
- Boundary conditions
  - Concentration or lateral influx of dissolved radionuclides at the boundaries
  - Concentration or lateral influx of particulate radionuclide at the boundaries for each sediment size fraction.

We are currently gathering flow, sediment and radionuclide data required by FETRA through search of both published and unpublished information at various sites. Table 3 shows nuclear power plants discharging or planning to discharge effluents to coastal waters. Available data for these plants are shown in Table 4. Additional data measured elsewhere are shown in Table 5. Particularly, data in the Irish Sea which receives a radionuclide effluent from the Windscale Nuclear Fuel Reprocessing Plant are shown in Table 6. The literature search indicates that Windscale and somewhat lesser extent, Hamboldt Bay Plants appear to have best available data. Based on the current information on available data, the Irish Sea was selected as the FETRA application site. We are now obtaining further information on measured flow-sediment-radionuclide data in the Irish Sea.

TABLE 3. Plants Discharging or Planning to Discharge Effluents to Coastal Waters (as of August 1, 1978)

Plant Name	Location	Utility	Commercial Operation	Net MWe	Water Body
Humboldt Bay 3	Eureka, CA	Pacific Gas & Electric	8/63	63	Pacific
Diablo Canyon 1, 2	Diablo Canyon, CA	Pacific Gas & Electric	3/78 10/78	1060 1060	Pacific
San Onofre 1	San Clemente, CA	Southern Cal. Edison, San Diego Gas & Electric	1/68	436	Pacific
(San Onofre 2, 3 - Plan to start operation in Oct. 80, Jan. 82, 1057 MWe each)					
Crystal River 3	Red Level, FL	Florida Power Corporation	3/77	825	Gulf
St. Lucie 1	Hutchinson Island, FL	Florida Power & Light, Corp.	12/76	802	Atlantic
(St. Lucie 2 - Plan to start operation in May 83, 802 MWe)					
Brunswick 1, 2	Southport, NC	Carolina Power & Light Co.	3/77	821	Atlantic
Millstone 1, 2	Waterford, CT	Northeast Utilities	12/70 12/75	652 828	Niantic Bay
(Millstone 3 - Plan to start operation in May 86, 1150 MWe)					
Pilgrim 1	Plymouth, MA	Boston Edison Co.	12/72	670	Cape Cod Bay
(Pilgrim 2 - Plan to start operation in June 85, 1180 MWe)					
Oyster Creek 1	Forked River, NJ	Jersey Central Power & Light	12/69	620	Barnegot Bay

TABLE 4. U.S. Nuclear Power Plants Located Along Coastal Zones - Available Data

Plant	References	Data Type	Radionuclides
Humboldt Bay 3	Heft, R.E. et al (1972)	Radionuclide concentrations in water and bed sediment	^{65}Zr, ^{65}Co, ^{137}Cs
		Description of physical features of bay and discharge canal	
	Noshkin, V.E. et al. (1976)	Dissolved radionculide concentrations	^{137}Cs, ^{134}Cs
		Particulate radionuclide concentrations (bed core samples, surface sediment sections)	^{137}Cs, ^{134}Cs, ^{54}Mn, ^{60}Co
	Harrison, F.L. et al. (1976)	Radionuclide concentrations (discharge canal) in water and bed sediment	^{54}Mn, ^{60}Co, ^{65}Zn, ^{137}Cs
	PG&E (1973)	Bathymetry data Hydrography information	
Maine Yankee	Churchill, J.H. (1976)	Particulate radionuclide concentrations (estuarine bed sediment)	^{137}Cs, ^{134}Cs, ^{58}Co, ^{60}Co, ^{54}Mn
		Sediment particle size dist.	
	Hess, C. (1979) Personal communiction	Other data to be made available (radionulcide concentrations - bottom sediment, hydrography, bathymetry)	
Oyster Creek 1	Blanchard, R.L. et al. (1976)	Particulate radionuclide concentrations (bottom sediment)	^{40}K, ^{54}Mn, ^{60}Co, ^{134}Cs, ^{137}Cs, ^{226}Ra, ^{125}Sb, ^{252}Th
		Sediment particle size dist.	
		Dissolved radionuclide concentrations	^{90}Sr, ^{137}Cs
		Particulate radionuclide concentrations (water samples)	^{54}Mn, ^{60}Co
Brunswick 1, 2 Crystal River 3 Millstone 1, 2 Pilgrim 1 St. Lucie 1 San Onofre	Environmental radiological monitoring reports	Dissolved rdionuclide concentrations (generally monthly grab samples Particulate radionuclide concentrations - bottom sediment (generally quarterly or semi-annual grab samples	
All of the above (except Crystal River 3)	Phillips, J.W. and J. Gruhlke (1977)	Dissolved radionuclide concentrations (in effluent)	^{58}Co, ^{60}Co, ^{90}Sr, ^{131}I, ^{134}Cs, ^{137}Cs ^{3}H

TABLE 5. Ocean Data

References	Water Body	Data Type	Radionuclides
Duursma, E. K. (1972)	Atlantic Mediterranean	Dissolved and particulate radionuclide concentrations	^{54}Mn, ^{59}Fe, ^{60}Co ^{65}Zn, ^{90}Sr, ^{95}Zr ^{106}Ra, ^{137}Cs, ^{144}Ce, ^{147}Pu
Duursma, E. K. and C. J. Bosch (1970)	Atlantic	Adsorption-desorption	Generic Study
Robbins, J. A. and D. N. Edgington (1975)	Great Lakes	Particulate radionuclide concentrations	^{137}Cs, ^{210}Ps, ^{239}Pu, ^{240}Pu
Jeffries, D. F. (1973)	British coastal waters	Dissolved and particulate radionuclide concentrations	^{137}Cs
Hetherington, J. A. (1976)	Irish Sea	Dissolved and particulate radionuclide concentrations	^{239}Pu, ^{238}Pu, ^{137}Cs
Livingston, H. P. and V. T. Bowen (1976)	Atlantic	Dissolved and particulate radionuclide concentrations	^{241}Am, ^{239}Pu, ^{230}Pu
Noshkin, V. E. (1972)	Atlantic	Radionuclide occurrence in marine sediment and biota	^{241}Am, ^{239}Pu, ^{137}Cs, ^{90}Sr
Noshkin, V. E. and V. T. Bowen (1973)	Atlantic and Mediterranean	Dissolved and particulate radionuclide concentrations	^{241}Am, ^{239}Pu, ^{240}Pu
Nevissi, A. and W. R. Schell (1974)	Bikini and Eniwetok Atolls	Dissolved and particulate radionuclide concentrations	^{240}Po, ^{239}Pu, ^{240}Pu
Nevissi, A. and W. R. Schell (1975)	Bikini and Eniwetok Atolls	Dissolved and particulate radionuclides concentrations	^{155}Eu, ^{207}Bi, ^{241}Am, ^{239}Pu, ^{240}Pu, ^{210}Pb
Nevissi, A. and W. R. Schell (1975)	Bikini and Eniwetok Atolls	Dissolved and particulate radionuclides	^{241}Am, ^{239}Pu, ^{240}Pu
Schell, W. R. (1973)	Bikini and Eniwetok Atolls	Dissolved and particulate radionuclides	^{241}Am
Schell, W. R. (1976)	Bikini and Eniwetok Atolls	Dissolved and particulate radionuclides	^{60}Co, ^{55}Fe, ^{207}Bi, ^{155}Eu, ^{241}Am, ^{239}Pu, ^{240}Pu, ^{235}U, ^{238}U
Schell, W. R. (1976)	Bikini and Eniwetok Atolls	Dissolved and particulate radionuclides	^{239}Pu, ^{240}Pu, ^{241}Am, ^{207}Bi, ^{155}Fu, ^{60}Co, ^{55}Fe, ^{210}Po
Silker (1972)	North Pacific	Dissolved and particulate radionuclide concentrations	^{7}Be, ^{106}Pu, ^{95}Zr-^{95}Nb, ^{144}Ce

TABLE 6. Windscale Plant Data

References	Data Type	Radionuclides
Dunster, H. J. et al. (1964)	Particulate radionuclide concentrations	^{90}Sr, ^{106}Ry, ^{144}Ce
Hetherington, J. A. and D. F. Jefferies (1974)	Particulate radionuclide concentration (estuarine and seabed sediments)	^{95}Zr/^{95}Nb, ^{106}Ru, ^{137}Cs, ^{144}Ce
	Particulate size distribution of sediment	
Hetherington, J. A. (1976)	Dissolved and particulate radionuclide concentrations	^{239}Pu, ^{238}Pu, ^{137}Cs,
Hetherington, J.A. et al. (1976)	Dissolved and particulate radionuclide concentrations	^{239}Pu, ^{240}Pu, ^{241}Am
Howells, H. (1966)	Particulate radionuclide concentration (shore silt, shore sand)	Total 6 (monthly) ^{106}Ru, ^{144}Ce, ^{137}Cs, (quarterly)
Mauchline, J. and W. L. Templeton (1963)	Dissolved radionuclide concentrations	^{106}Ru, ^{144}Ce, ^{137}Cs, ^{95}Sr/^{95}Nb, ^{90}Sr
	Hydrography information	
Templeton, W. L. and A. Preston (1966)	Particulate radionuclide concentration (seabed)	^{106}Ru, Pu, ^{137}Cs, ^{90}Sr
	Particulate radionuclide concentration (estuarine silt)	^{106}Ru, ^{144}Ce, ^{95}Zr/^{95}Nb
	Concentration in unfiltered sea water	^{106}Ru, ^{90}Sr
	Dissolved radionuclide concentration (filtered sea	^{106}Ru, ^{144}Ce, Pu, ^{95}Zr/^{95}Nb, ^{90}Sr, ^{137}Cs
	Seabed composition in area Hydrography information	

TASK C. TRANSPORT OF SEDIMENT AND RADIONUCLIDES IN ESTUARIES

We are currently synthesizing a three-dimensional model for sediment-radionuclide transport model for estuaries. The model can also calculate hydrodynamics and temperature salinity transport. Several computer runs were made to examine the usable aspect ratio (ratio of length to width to height) of each computational cell. Usable aspect ratios were examined by computing the flow pattern in a rectangular waterbody with the upstream velocity of 2.0 ft/sec, as shown in Figure 3. The first case has an aspect ratio of 1 (vertical direction Y): 10 (lateral direction Z):100 (longitudinal direction X). The variation of computed longitudinal velocities (U) along Y = 5.5 ft and Z = 25 ft at X = 100 ft, 200 ft, 300 ft, 400 ft, and 500 ft are shown in Figure 4. The vertical variation of computed longitudinal velocities along Z = 25 ft at these five locations are shown in Figure 5. These figures indicate that distributions of longitudinal velocities are almost uniform both longitudinally and vertically.

The second case has an aspect ratio of 1 (Y direction):300 (Z direction): 10,000(X direction). Computed longitudinal velocities (U) at X = 10,000 ft, 20,000 ft, 30,000 ft, 40,000 ft, and 50,000 ft are shown in Figures 6 and 7. Figure 7 indicates that vertical velocity distributions are no longer uniform because the boundary layer formed along the bottom surface is reducing the velocity near the bottom and consequently increasing the velocity near the water surface. The further the longitudinal distance, the more this trend shows, as clearly indicated in Figure 6. These two cases demonstrate that the three-dimensional model can handle very large aspect ratios of computational cells. To be able to use a large aspect ratio is essential to any three-dimensional model if a model must have a practical usage to estuarine radionuclide modeling.

The next test was to simulate wind-driven circulations in a 3400 m-long, 1400-m wide and 7-m deep rectangular water basin with a diagonal wind of 18 m/sec blowing on the water surface as shown in Figure 8. This case was selected as a test case because Leendertse et al. (1973) reported their computation results by using their quasi-three dimensional model which requires

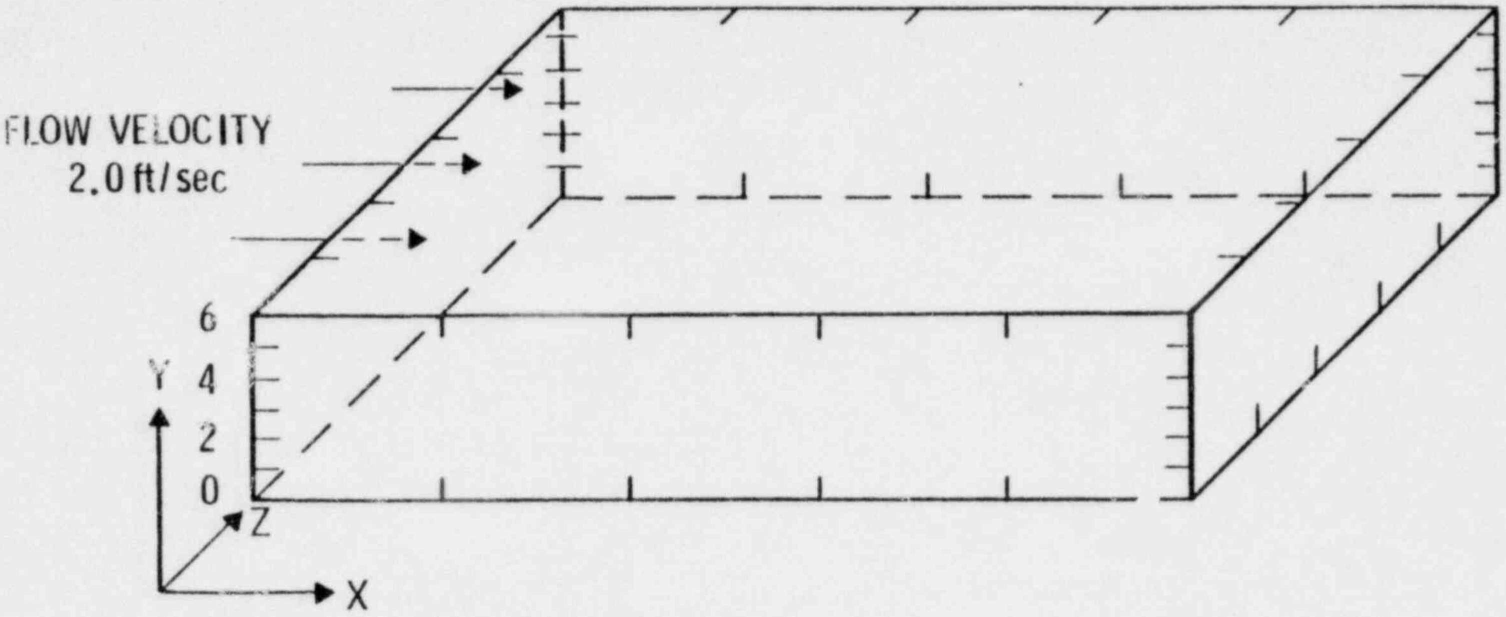

FIGURE 3. Rectangular Waterbody Used for the Examination of the Aspect Ratio

1:10:100 ASPECT RATIO

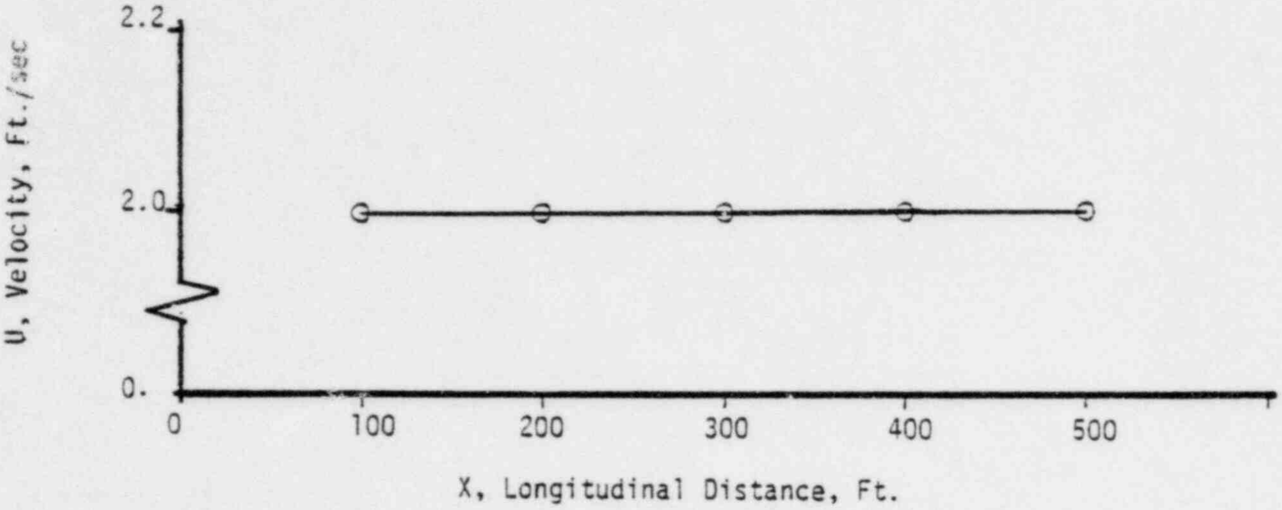

FIGURE 4. Variation of Longitudinal Velocities Along Y = 5.5 ft and Z = 25 ft

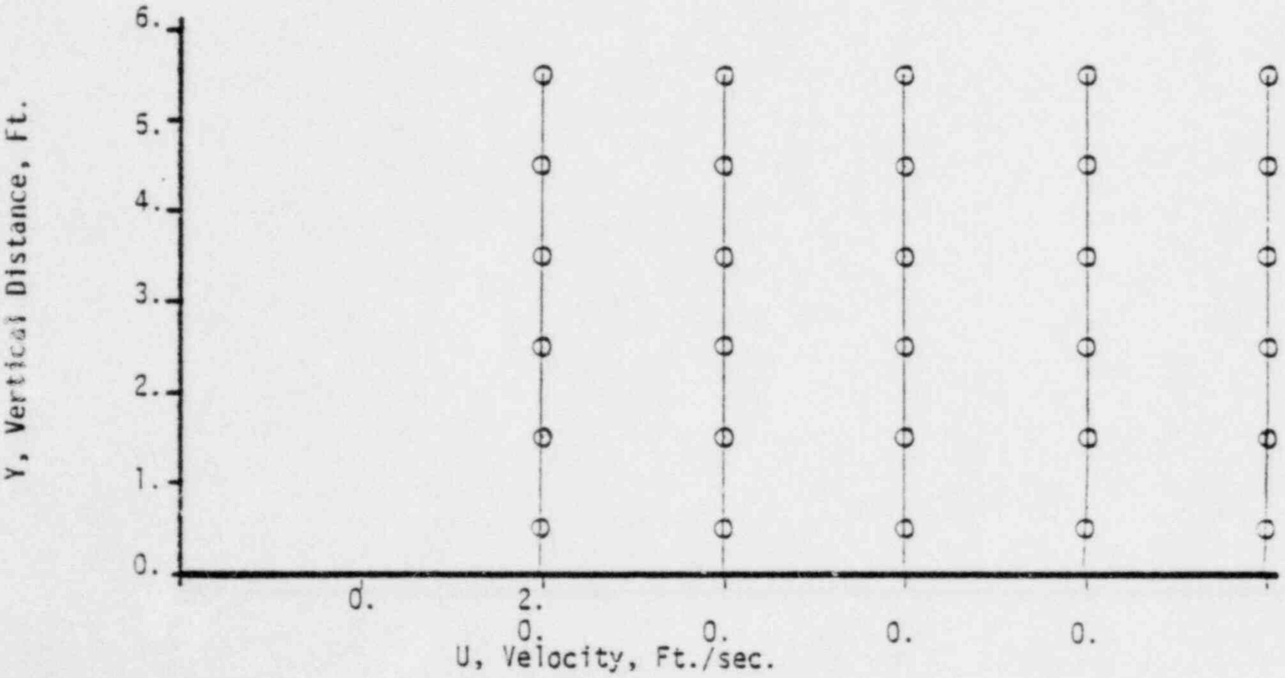

FIGURE 5. Vertical Variation of Longitudinal Velocities Along Z = 25 ft

1:300:10000 ASPECT RATIO

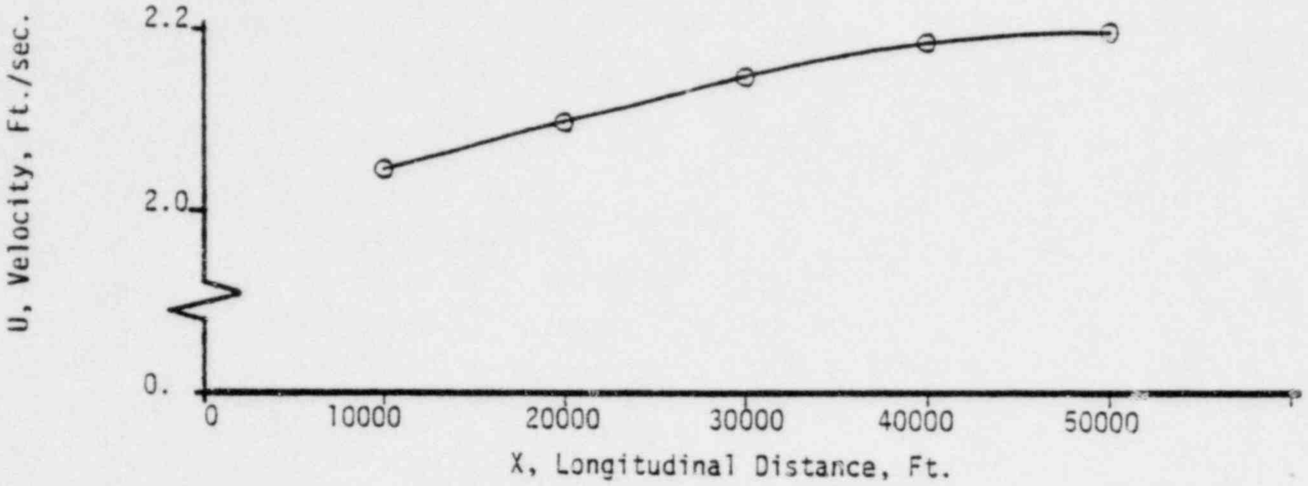

FIGURE 6. Variation of Longitudinal Velocities Along Y = 5.5 ft and Z = 750 ft

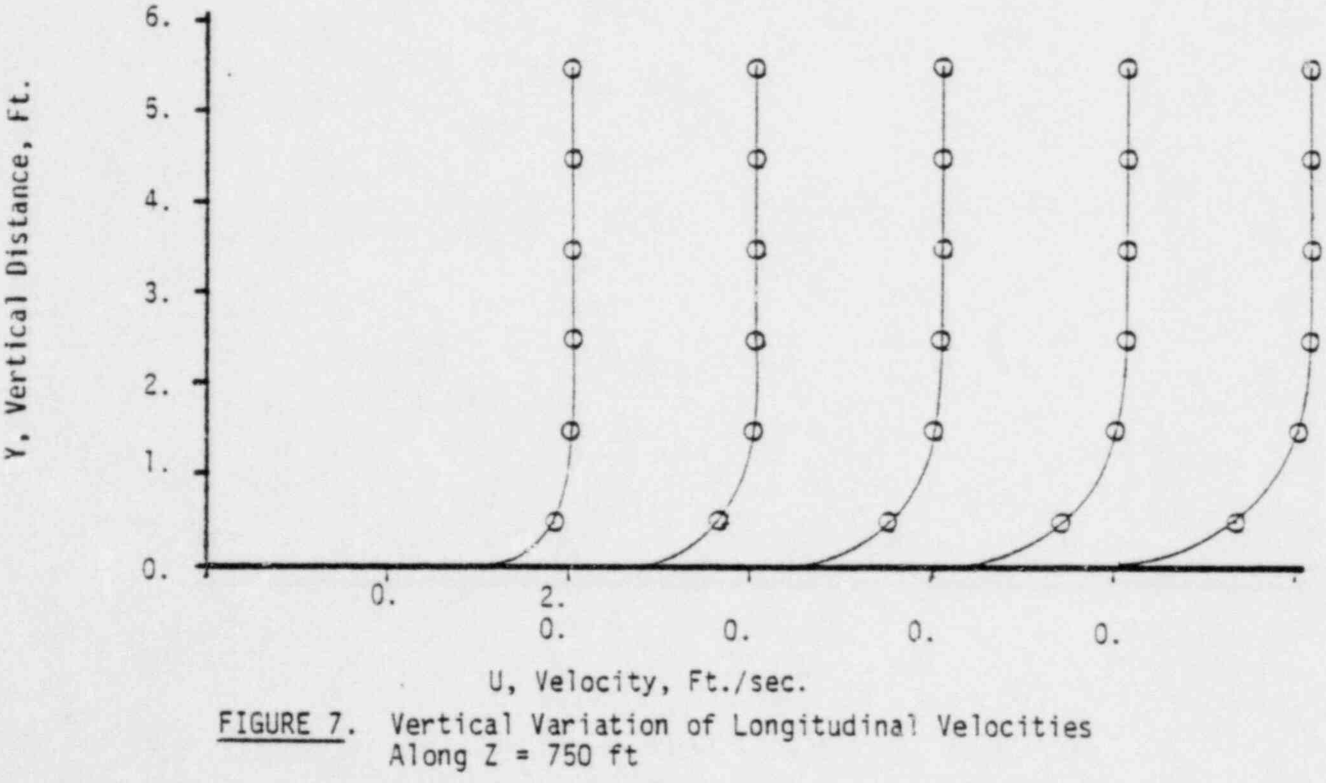

FIGURE 7. Vertical Variation of Longitudinal Velocities Along Z = 750 ft

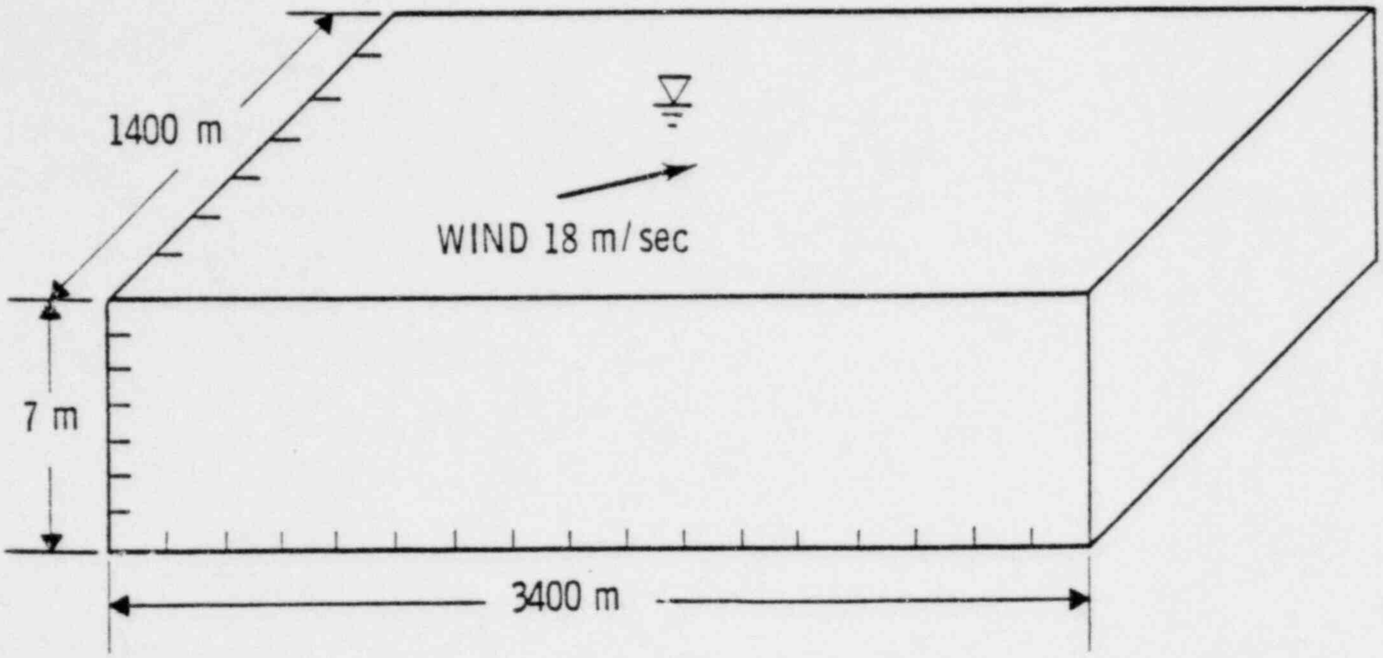

FIGURE 8. Water Body Used for the Wind-Driven Circulation Computation

the aspect ratio of longitudinal and lateral directions to be 1:1. Computed results by our three-dimensional model is shown in Figure 9 at the time of 375 sec. Figure 9a indicates the flow pattern on the vertical section along the center, while other figures show the horizontal patterns at seven different elevations. These figures indicate a large basin-wide circulation induced by the wind. Computed results by the Leendertse's model are shown in Figure 10. Comparison of Figures 9 and 10 indicates that agreement between these model results are good.

Literature review on available data for the estuarine environment indicates that the Hudson River estuary (along where the Indian Point Nuclear Power Plant is located) and Montsweag Bay (along where the Main Yankee Nuclear Power Plant is located) are two of the best model application sites. We are currently obtaining further information on these two sites to select an estuarine modeling site for this study.

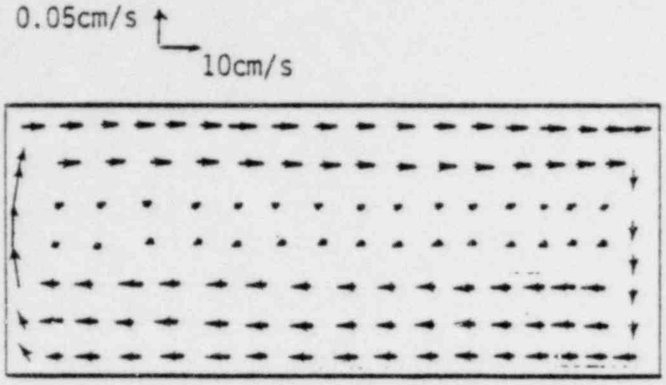

FIGURE 9a. at 375 sec: Vertical Section along the Center

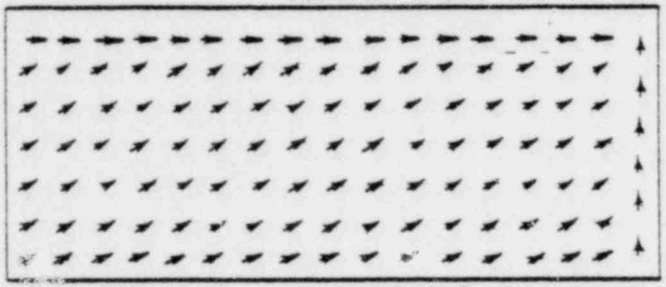

FIGURE 9b. Horizontal Section: Top (6.5m)

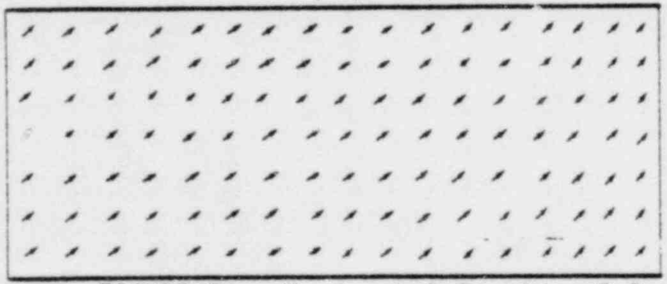

FIGURE 9c. Horizontal Section: 5.5m

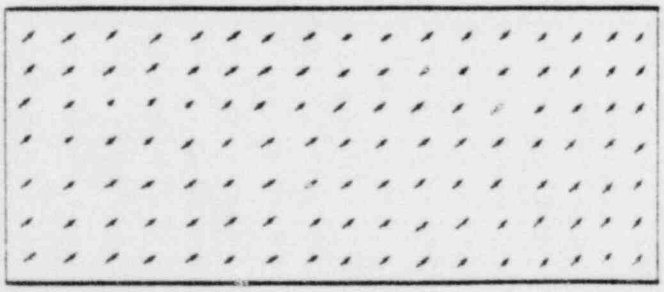

FIGURE 9d. Horizontal Section: 4.5m

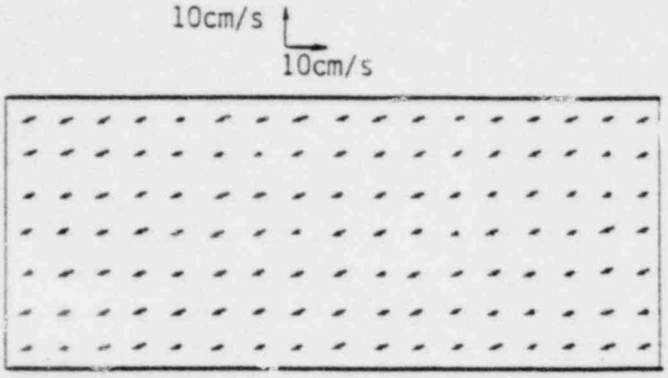

FIGURE 9e. Horizontal Section: 3.5m

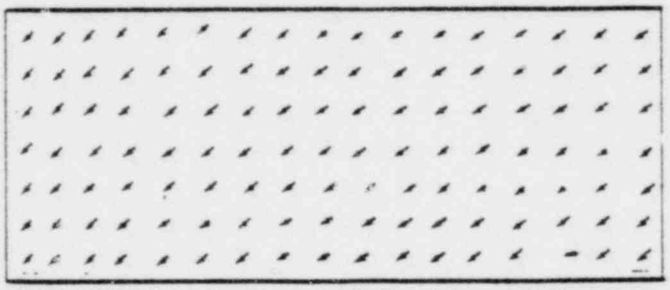

FIGURE 9f. Horizontal Section: 2.5m

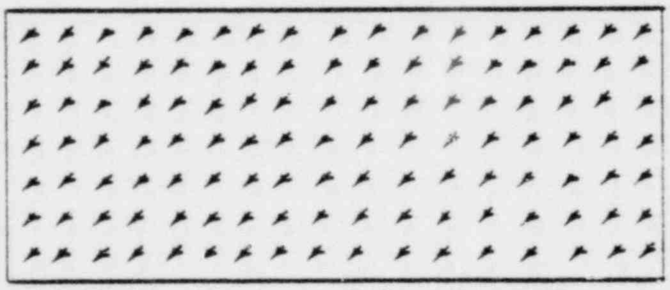

FIGURE 9i. Horizontal Section: 1.5m

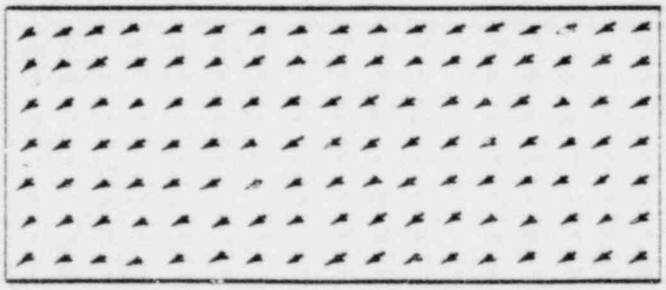

FIGURE 9j. Horizontal Section: Bottom (0.5m)

FIGURE 9.

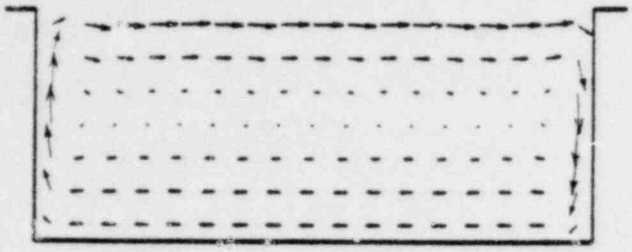

FIGURE 10a. at 375 sec: Vertical Section cut through Center

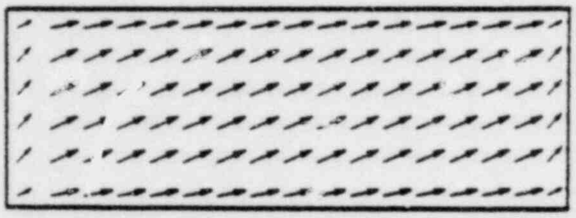

FIGURE 10b. Horizontal Plane, Layer 1 (Surface)

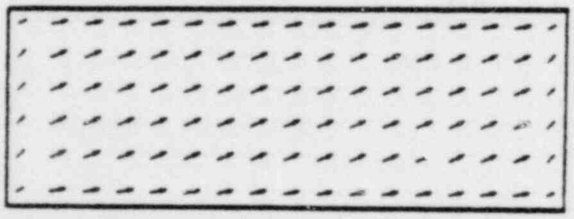

FIGURE 10c. Horizontal Plane, Layer 2

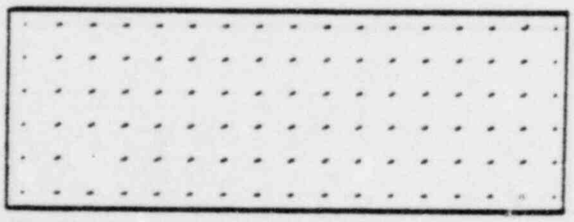

FIGURE 10d. Horizontal Plane, Layer 3

FIGURE 10e. Horizontal Plane: Layer 4

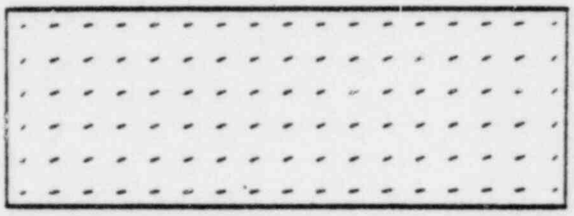

FIGURE 10f. Horizontal Plane, Layer 5

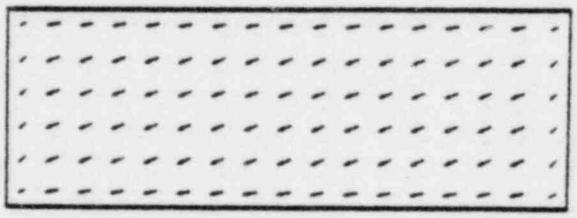

FIGURE 10i. Horizontal Plane, Layer 6

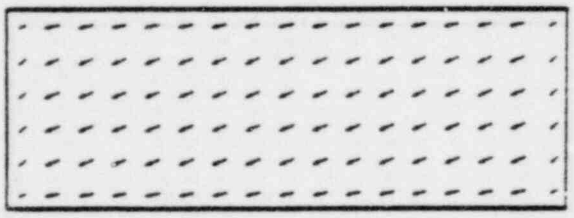

FIGURE 10j. Horizontal Plane, Layer 7 (Bottom)

FIGURE 10. Velocity Components in a Cross-Section and in Seven Horizontal Layers of a Wind-Driven Rectanular Basin at 375 Second of the Computation by the Leendertse's Model

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