Technical Report CERC-94-4
February 1994

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US Army Corps
of Engineers
Waterways Experiment
Station

New York Bight Study

Report 3
Three-Dimensional Particle Tracking Model for Floatables and Dissolved and Suspended Materials

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Prepared for U.S. Army Engineer District, New York

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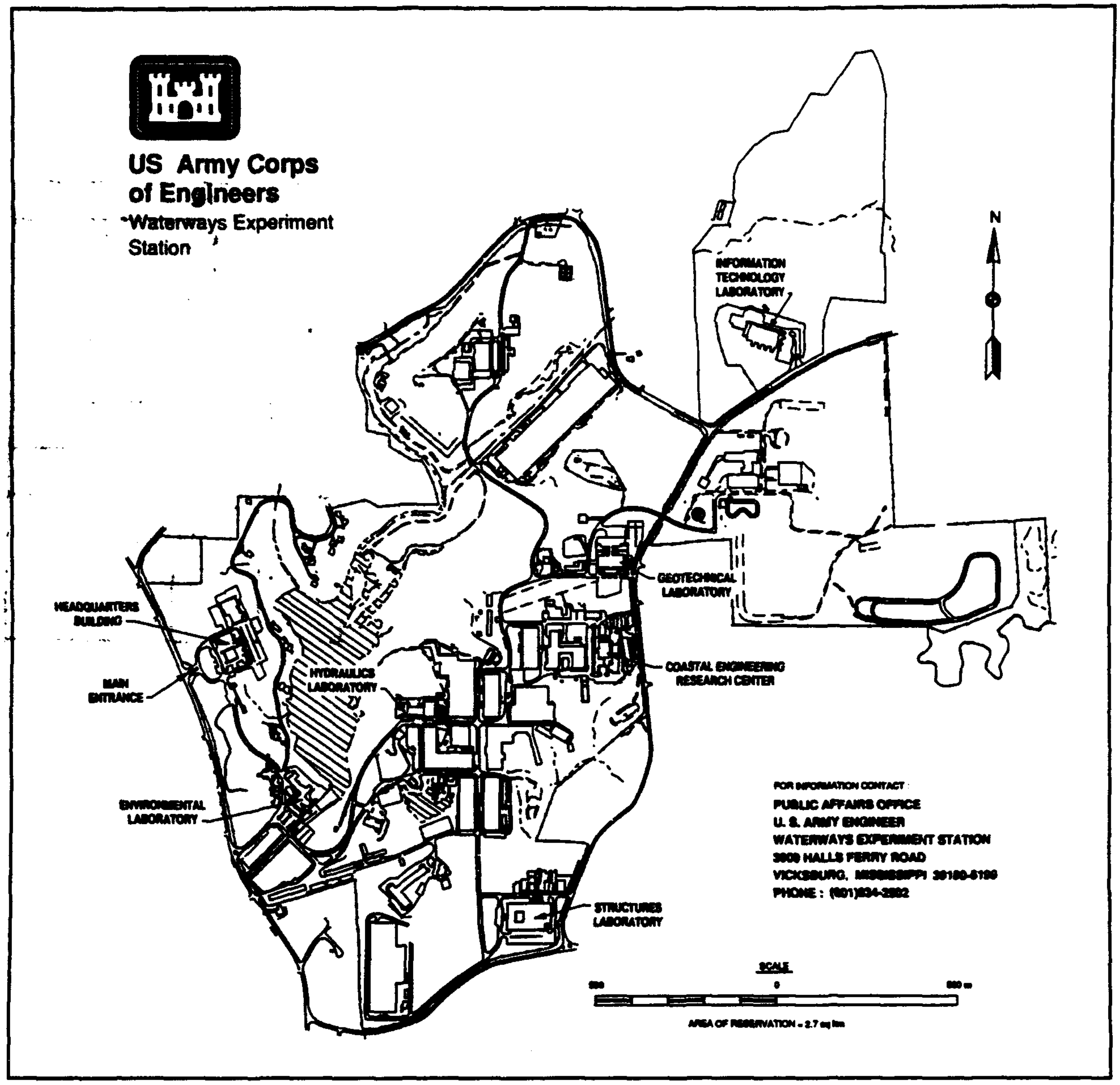

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Contents

Preface

The work described herein was conducted by Dr. Raymond Chapman of Ray Chapman and Associates, Vicksburg, MS, for the U.S. Army Engineer Waterways Experiment Station (WES), under Contract No. DACW39-92-C-00-14. Mr. Terry K. Gerald of AScI, Inc., developed the interactive interface software. The contract was monitored by Dr. Mark S. Dortch, Chief, Water Quality and Contaminant Modeling Branch, Environmental Laboratory (EL), WES. Support for this work was provided by the U.S. Army Engineer District, New York, under the Water Resource Development Act of 1986 (Public Law 96-662, Section 728a).

This report was prepared by Dr. Chapman, Mr. Gerald, and Dr. Dortch under the general supervision of Mr. Donald L. Robey, Chief, Environmental Processes and Effects Division, EL, and Dr. John Harrison, Director, EL.

At the time of publication of this report, Director of WES was Dr. Robert W. Whalin. Commander was COL Bruce K. Howard, EN.

1 Introduction

Within the scope of the Water Resource Development Act of 1986 (PL 96-662, Sec. 728a), a feasibility study was authorized for the purpose of developing a monitoring and modeling strategy for water quality management of the New York Bight. As part of the overall modeling strategy, a numerical model capable of predicting the transport and fate of floatables and suspended or dissolved materials using a three-dimensional (3D) particle tracking methodology was developed. Specific features implemented include (a) surface transport of floatables by the wind, and (b) 3D advection and diffusion of suspended and dissolved matter. The particle tracking model is interfaced with the U.S. Army Engineer Waterways Experiment Station's 3D hydrodynamic model (CH3D) (Johnson et al. 1991). In addition, interactive window-based software has been developed to assist in the setup and operation of the stand-alone version of the particle tracking model. This report presents the particle tracking model development and verification. It is one of five reports of the New York Bight Study.

2 Model Formulation

Particle tracking within the CH3D boundary-fitted model is performed on the transformed grid to take advantage of the unit square computational cells. Particle positions x_i are updated from time level N to $N + 1$ as follows:

$$x_i^{N+1} = x_i^N + \Delta x_i^N \tag{1}$$

where the transformed contravariant particle displacement vectors are approximated via the following second-order Taylor series:

$$\Delta x_i = u_i \Delta t + \frac{du_i}{dt}\frac{\Delta t^2}{2} \tag{2}$$

where

Δx_i = displacement vector

u_i = contravariant velocity vector

t = time

and

$$\frac{du_i}{dt} = \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} \tag{3}$$

At the end of a desired output interval, the contravariant position vectors are transformed to Cartesian coordinates and stored along with grid cell indices for graphical display purposes.

Specific issues addressed during the development of a CH3D-based particle tracking model were boundary conditions, the required accuracy of the spatial interpolation and temporal integration schemes, wind-generated surface current and wave drift, model verification, and the mode of operation of the particle tracking routine.

The required accuracy of the spatial interpolation and temporal integration schemes were examined by testing alternative versions of the particle tracking model. The interpolation of the velocity components within the 3D grid is accomplished by either a bilinear or biquadratic interpolation on each horizontal grid cell and a two point interpolation between vertical layers (Hildebrand 1956). Shift operators are employed to properly orient the unit square interpolation functions on the space-staggered hydrodynamic grid. The temporal integration options for Equation 2 are a first-order Euler and a second-order trapezoidal (Henrici 1964). When the second-order time integration options are employed, an additional option is provided to either include or omit the CH3D convective acceleration vector (FI,FJ) in computation of the particle trajectory (Equation 3).

Depending on the selection of the vertical grid spacing, the near-surface velocities predicted by CH3D can be several meters below the free surface. As a consequence, an Ekman surface current extrapolation (Neumann and Pierson 1966) is required to estimate the surface drift required for floatables. The extrapolation technique is based on Ekman surface drift velocity profiles which read as follows:

$$V_x(z) = V_o e^{-\alpha z} COS(\beta z) \tag{4}$$

and

$$V_y(z) = V_o e^{-\alpha z} SIN(\beta z) \tag{5}$$

where

V_x = X velocity component

V_o = surface drift velocity

α = decay factor with depth z

β = rotation factor with depth z

V_y = Y velocity component

Specifically, the magnitude and direction of the surface velocity V_o is computed by simply fitting the decay and rotation factors using the velocity components (V_x, V_y) defined within the top two CH3D grid cells.

The wind-forcing methodology adopted for floatables is based on a balance of the aerodynamic and hydrodynamic forces exerted on a floating object and the object's acceleration. The balance equation for the X component of particle motion is as follows:

$$\frac{\partial U_p}{\partial t} = fV_p + F_a + F_w \tag{6}$$

where

U_p = X component of the wind-driven particle velocity

f = Coriolis parameter

V_p = Y component of the wind-driven particle velocity

F_a = combined shear and form drag force of the wind

F_w = combined shear and form drag force of the water

A quadratic drag law is adopted for the contribution of shear and form drag forces. As a result, wind forces per unit mass are written as follows:

$$F_a = \frac{\rho_a}{\rho_p}\left(\frac{C_f}{H} + \frac{C_d}{L}\right)U_{ar}Q_{Ar} \tag{7}$$

where,

$\rho_{a,p}$ = air and particle density

$C_{f,d}$ = skin friction and form drag coefficients

H = nominal particle height

L = nominal particle length

U_{ar} = relative wind speed, $U_a - U_p$

Q_{ar} = resultant relative wind speed

An identical force formulation is used for the water forces with the exception that water and particle densities are used and the sign of the relative particle speed is changed. Using the surface velocities estimated by the Ekman extrapolation subroutine, Equation 6 is integrated to obtain velocity used to update the *X* trajectory displacement equation (first term on right side of Equation 2) in the particle tracking subroutine. The second term on right side of Equation 2 is not used for floatables. A similar equation for the *Y* component velocity has also been implemented. In addition to the direct wind force balance, the influence of wave-induced transport (i.e., stokes drift) is included by adding 1.5 percent of the wind speed to the surface particle velocity (Kenyon 1969).

Subroutine WFORCE, which estimates the wind-driven transport, is called by the particle tracking subroutine each time step. The switches IFLT, ISURF, and IWIND are set to one to enable the call to WFORCE. Data that are read into the particle tracking routine are the skin friction and form drag coefficients for air and water, the nominal height and length of the particle, and the fraction of the particle height that is exposed to direct wind forcing.

With regard to particle settling, a single settling velocity representative of the mean particle size or density is specified. Subsequent to nondimensional scaling, the constant settling speed is simply subtracted from the interpolated vertical velocity prior to the particle position update. At the present time, when a particle reaches the bottom, it remains there.

Particle diffusion is assumed to follow a simple random walk process (Fischer et al. 1979). Specifically, a diffusion distance defined as the square root of the product of an input diffusion coefficient and the time step is decomposed into *X* and *Y* displacements via a random direction function. The *Z* diffusion distance is scaled by a random positive or negative direction. The equations for the horizontal and vertical diffusion displacements are written as follows:

$$L_x = \sqrt{D_h \Delta t}\, COS(2\pi R) \tag{8}$$

$$L_y = \sqrt{D_h \Delta t}\, SIN(2\pi R) \tag{9}$$

$$L_z = \sqrt{D_z \Delta t}\,(0.5 - R) \tag{10}$$

where

L_x = X direction diffusion distance

D_h = horizontal diffusion coefficient

R = random real number generator between 0.0 and 1.0

L_y = Y direction diffusion distance

L_z = Z direction diffusion distance

D_z = vertical diffusion coefficient

Subsequent to the above computations, the diffusion distances are then scaled and added to the particle update equation (Equation 1) each iteration.

The implementation of the particle tracking model into the CH3D hydrodynamic simulation of the New York Bight required boundary option development. Boundary options were developed for land and the seaward boundary. Two options are available for land boundaries and are specified by means of the parameter IBND. When IBND is set to zero, a particle will remain on land when it intersects a land boundary. In this case, the parameter ISWC is reset from zero, an active particle, to one, an inactive particle, which is removed from the computation. A value of one for IBND allows a particle to slide along a land boundary and remain within the computational grid. Inflow and outflow options are available for seaward or water boundaries. A particle approaching a seaward boundary passes through the boundary and is removed from the computation by setting the parameter ISWC to one. If desired, inflow boundaries can act as multiple continuous release points. This feature is controlled by the parameters ICON, IFRC, and NPAR. The limitation of this option is that it only works for point continuous releases, which means that grid-wide initial particle positions cannot be specified.

The particle tracking model has two operational options. The first includes the particle tracking model as subroutines within CH3D. In this mode, the particle trajectory computations are performed in concert with the hydrodynamic simulation, and the display of particles is conducted during postprocessing. The second mode performs the particle tracking computations within a stand-alone graphics program that allows simultaneous simulation and animation of particle movement. When the stand-alone version of the particle tracking model is used, CH3D is run independently and the time-invariant geometric data that defines the grid are stored along with temporally averaged (e.g., 1-hr average) velocity components. This mode has the advantage that various particle release points can be easily and quickly evaluated using preprocessed hydrodynamics. Thus, various gaming analyses can be conducted such as deriving impact probabilities utilizing multiple particle release positions.

3 Stand-Alone Particle Tracking Model

The basic idea behind the stand-alone particle tracking model and graphical interface is that CH3D hydrodynamic simulations are performed independently where time-invariant geometric information is stored along with temporally averaged wind speeds, surface drift currents, surface elevations, and 3D velocity components for each grid cell location. A description of the CH3D hydrodynamic variables can be found in Johnson et al. (1991).

To preserve wind speed information in subroutine CH3DWT, two additional arrays have been added to CH3D and the common block CH3D.INC. The arrays TXF and TYF save the time interpolated values of the dimensional Cartesian wind speeds. The arrays TXFL and TYFL contain the dimensional transformed components of the wind speed. The wind speed data saved in the TXFL and TYFL arrays are used by the floatable force balance subroutine WFORCE in both the particle tracking subroutines and the stand-alone particle tracking model. These data are written to a disk file during the CH3D model run by subroutine WQPM. Stand-alone particle tracking simulations are then performed using the windows interface software that sets up and executes the particle tracking routine PARS and the graphical output routines.

The output subroutine WQPM is run as part of CH3D during a hydrodynamic simulation. The inputs to WQPM (File 90) are the averaging interval NAVG and the output starting iteration ITWQS. The output from WQPM (File 70) are (a) time-invariant transformation data that geometrically relate the physical grid system to the transformed computational grid, and (b) time-varying, time-averaged hydrodynamic data (File 71). The time-invariant data are output once and consist of nondimensional scaling parameters (UREF, XREF, ZREF, and RB), the nondimensional hydrodynamic simulation time step (DT), spatial transformation derivatives (X1, X2, Y1, and Y2), metric tensors (G11, G12, G22, and GD), and grid row and column reference quantities (NROW, IROW, IU1, IU2, NCOL, JCOL, JV1, and JV2). This operation occurs when WQPM is first called by CH3D, or when the time iteration counter IT equals ITWQS.

During each CH3D iteration subsequent to ITWQS, surface velocities (USRF and VSRF) are computed using the Ekman surface drift subroutine

EK2, and averages of the hydrodynamic field information (UA, VA, WA, FIA, FJA, TXFLA, TYFLA, and AHSSA) are accumulated. At the end of averaging interval NAVG, the particle tracking hydrodynamic output is written to File 71, and the arrays are reset to zero.

Extensive testing of the various particle tracking options has shown that the small amount of additional computational effort required by the higher order interpolation and integration is warranted when compared with the additional accuracy gained. As a consequence, the particle tracking options selected for use in the stand-alone particle tracking model (PARS) are (a) second-order trapezoidal rule time integration, (b) biquadratic spatial interpolation over each horizontal grid cell with a two point vertical interpolation, (c) nonlinear horizontal convective acceleration, (d) Ekman surface drift, (e) direct wind forcing on floatables, (f) constant speed particle settling, (g) isotropic particle diffusion, and (h) single and multiple position, instantaneous and continuous particle releases.

A graphical user interface providing a point and click operating environment has been created to aid the user in the operation of the stand-alone particle tracking model. The user may start the interface by typing in "pt" from the directory containing the graphical user interface software. This interface provides a main control panel from which the user may perform input and model execution tasks (Figure 1). Prior to execution of the model, two input tasks are performed: (a) specification of particle release sites, and (b) input of model control parameters. While specifying a sequence of release sites, the main control panel allows the user to either create a file containing new release sites and types (ie., single, multiple, and continuous particle releases) or select a pre-existing file. Whenever the user elects to create a new release site file, a window will appear, containing an image of the New York Bight grid, that allows the user to point and click the location of release sites (Figure 2). A listing of existing release site files can be generated via pushbutton on the main control panel. This allows the user to select and graphically view a particular release site. The user is also provided with the capability of deleting a release site file with the release site manager pushbutton.

Specification of model input control parameters such as particle density, drag coefficients, and wind-forcing-enabled is accomplished through interaction with the main control panel. The create pushbutton allows the user to create a new control parameter file. A dialog window with a listing of control parameters, default settings, and help pushbuttons will appear on the screen (Figure 3) when the user selects the create pushbutton. The help pushbutton provides detailed information on each parameter. All control parameters are forced to have a specified range of values. If the user attempts to set a parameter to a value outside its allowable range, it will be reset to its default value and a warning dialog window will appear. The user is also provided with the ability to view and edit an existing control parameter file by clicking on the control parameter file view pushbutton. The user is provided the option to delete an existing control parameter file by clicking on the control parameter manager pushbutton.

The final task consists of creating and viewing the particle trajectory output file. To create a trajectory file, the user will execute the model by clicking on the trajectory file create pushbutton. A dialog window prompting the user for the particle tracking trajectory file will appear. Once the user selects a filename, another window will pop up containing two file selection dialogs (Figure 4). The user must then select a release site and parameter control file to continue. Once this has been done, the model is executed. During model execution, a window is displayed that provides a model run status field and an abort pushbutton.

Subsequent to model execution, the user may view the trajectory output by clicking on the trajectory file view pushbutton on the main control panel. This provides a file selection dialog window prompting the user to select a trajectory file. Next, a window will appear that allows the user to view an animation of the particle trajectories (Figure 5).

The particle tracking model's graphical user interface software was written using a combination of X-windows and the Silicon Graphics' graphical programming library GL. Its use is limited to computer platforms supporting both software packages such as the Silicon Graphics workstation used during software development.

4 Model Verification

The initial set of test simulations consisted of comparing particle trajectory results with the analytical solution of Lagrangian residual currents in a two-dimensional (longitudinal-vertical) dead-end tidal channel of constant width, depth, and density (Ianniello 1977). The CH3D model setup included constant density, no wind stress, a linear bottom shear, a constant 21.7-cm^2/sec eddy viscosity, and a simple 12.42-hr period tide. The rectangular grid was 20 cells long, 10 cells deep, and 1 cell wide with grid spacings of Δx = 3.5 km, Δz = 1.0 m, and Δy = 3.5 km. The purpose of the test was to determine if the particle tracking schemes predicted the correct residual transport within the channel. A single particle was initially released in each of 10 vertical layers and tracked for 1 tidal cycle subsequent to a 10-tidal cycle spin-up. The residual velocity was then computed by dividing each particle displacement from the initial longitudinal position by the tidal period. The results of the first-order, bilinear particle track test computation are presented in Figure 6, in which the predicted Lagrangian residual velocity is compared with the analytic solution (Ianniello 1977) at a location 7 km from the tidal boundary. Examination of the figure shows close agreement between model and analytic solution.

Drogue trajectory data collected by the U.S. Environmental Protection Agency (EPA) for the years 1989 through 1991 were examined to determine if surface trajectories data were available within the New York Bight hydrodynamic model grid.[1] Of the more than 50 drogue trajectory files provided by EPA, only 1 contained drogue positions that resided within the grid for an adequate enough time to perform a model comparison. This surface drogue entered the computational grid from the east on 22 April 1991 and exited to the southwest around 22 May 1991. During this time period, the surface drogue moved from 40.2 N, 70.4 W to 38.5 N, 73.5 W.

Wind speed and direction data during the simulation period were obtained for Kennedy International Airport, Ambrose Light, and two National Oceanic and Atmospheric Administration (NOAA) data buoys. Kennedy International (KI) and Ambrose Light (AL) lie north and west of the drogue trajectory with coordinates 40.5 N and 73.8 W. NOAA data buoy Station 12 is located at

[1] Personal Communication, 1992, D. Pabst, EPA 106-Mile Drifting Buoy Study Project Manager, Washington, DC.

38.8 N and 74.6 W, which is west and south of the drogue path. NOAA data buoy Station 4 is located south and west of the drogue trajectory at coordinates 39.0 N and 70.0 W.

To determine which meteorological data set or combinations of data sets should be used to drive the particle tracking model, hourly data for paired locations were plotted against one another (Figures 7-12). Examination of these figures leads to a number of observations. The most obvious and troubling observation is that there is very little correlation or consistency between stations. For example, a comparison of wind speed and direction between Ambrose Light and Kennedy International (Figures 7 and 8) shows that the wind speed at Ambrose Light is normally greater than that at Kennedy. This might be attributed to an over-land versus over-water wind effect, and there is considerable scatter in the observed directions. A comparison of an offshore and nearshore station, NOAA data buoy 4 and Ambrose light, shows that the nearshore wind speeds are usually greater than that observed offshore (Figure 9). Although the wind directions in an average sense appear to be similar, there is considerable scatter in the hourly measurements (Figure 10). Finally, a comparison of the NOAA data buoys 4 and 12 (Figures 11 and 12) shows that the offshore wind speeds are comparable, but again there is scatter in the measured directions.

Wind data for the time period 22 April to 22 May 1991 were available at Kennedy International, Ambrose Light, and NOAA data buoy 12. Model predictions utilizing wind speeds and directions from these stations did not compare well with the observed trajectory. For example, the predicted particle trajectory (dashed line) using NOAA data buoy 12 is compared with the drogue observations (solid line) in Figure 13. In this figure, the open box denotes the starting position and the closed circles denote the end position. It is seen in this figure that both the predicted mean direction and total distance traveled are not predicted well. The inability of the model to accurately predict the drogue trajectory using any of the available individual wind data can be attributed to (a) the remoteness of the wind data sets stations from the trajectory positions, and (b) the lack of uniformity of the grid wide wind field as exhibited by the lack of correlation between wind stations.

In an attempt to generate a wind field that is more representative of the large scale or geostrophic wind variability during the simulation period, mean wind speeds and directions were determined from the offshore stations after all short duration or localized storm events were removed. In other words, only mean wind and directions that persisted for a day or more were included in the constructed wind field. A repeat of the particle tracking simulation using the constructed wind field resulted in a predicted particle trajectory that more reasonably mimicked the observed data. Table 1 lists the observed and predicted latitude (N) and longitude (W) drogue trajectory positions, respectively. In this table, simulation day zero corresponds to midnight on 23 April 1991. Figures 14 and 15 provide correlation plots of the data presented in Table 1.

Table 1
Comparison of Observed and Predicted Drogue Trajectory Positions

	Observed		Predicted	
Simulation Day	**N**	**W**	**N**	**W**
0	40.18	70.42	40.18	70.42
4	40.21	71.04	40.21	71.09
5	40.17	71.20	40.20	71.23
7	40.12	71.47	40.20	71.49
10	39.92	71.86	39.90	71.89
12	39.72	72.17	39.79	72.14
15	39.53	72.48	39.55	72.50
18	39.23	72.79	39.30	72.80
23	38.98	73.05	38.98	73.13
27	38.75	73.50	38.76	73.37

5 Conclusions and Recommendations

At the present time, the implementation of the particle tracking model is complete. Additional improvements that could enhance the predictive capability of the particle tracking model are (a) a "puff" or near field outfall source algorithm, (b) statistical representation of particle size or density for differential settling analyses, (c) anisotropic particle diffusion that varies with the spatial scale of the release, and (d) near-bottom bedload transport because of currents and waves.

With respect to floatables prediction, given that the offshore transport of floatables is controlled almost entirely by the local winds, it is imperative that an accurate characterization of both the mean wind speed and direction is used to drive the particle tracking model. Consequently, if winds remote to the area of interest must be used in the particle tracking simulation, care should be taken to remove localized storms or variability from the wind record. If possible, barometric pressure charts (ie., kinematic analysis; Cardone 1969; Cardone, Greenwood, and Greenwood 1992) should be used in conjunction with the point wind measurements to ensure that the long-term variations in mean wind speed and direction are represented in the applied wind field.

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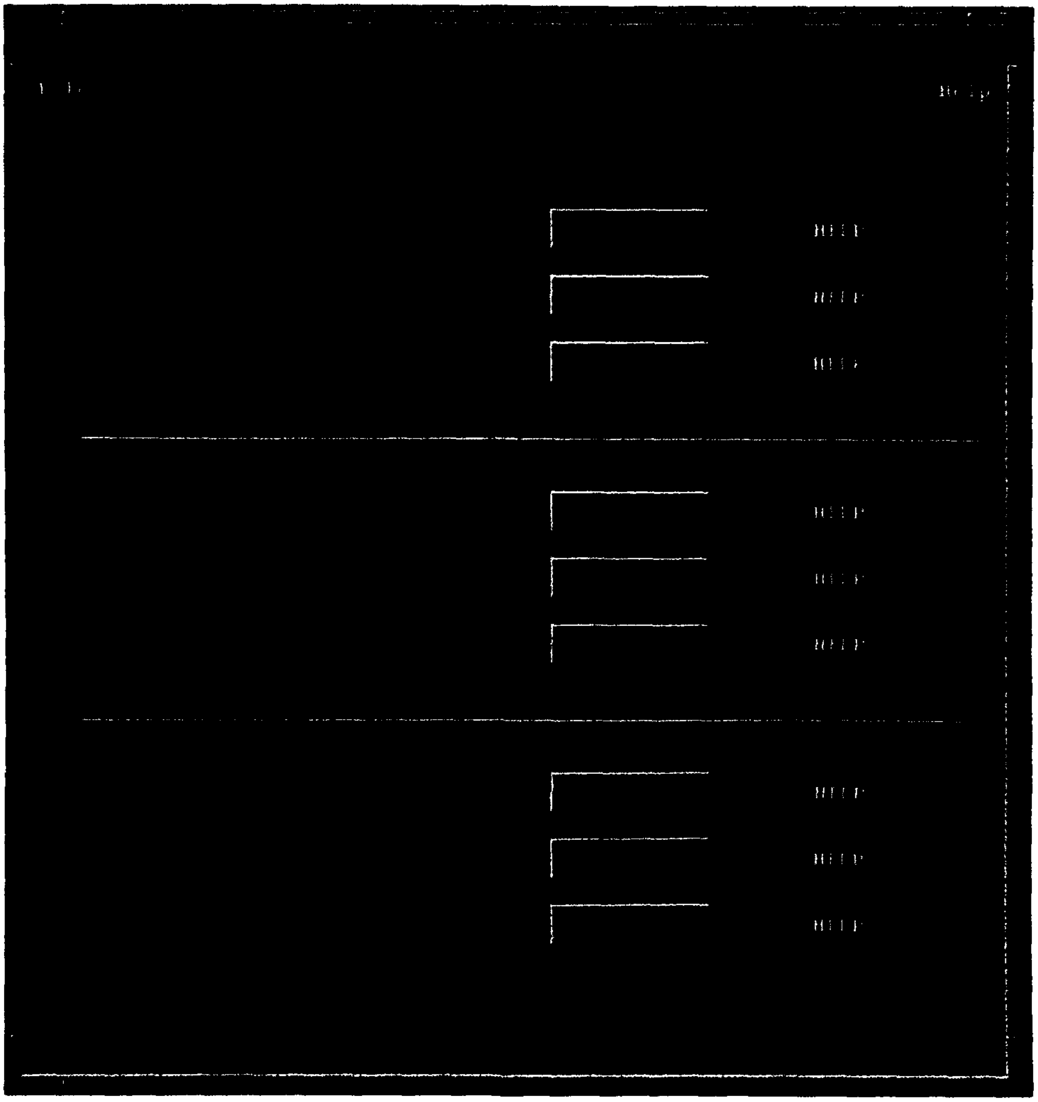

Figure 1. **Main control screen for the user interface**

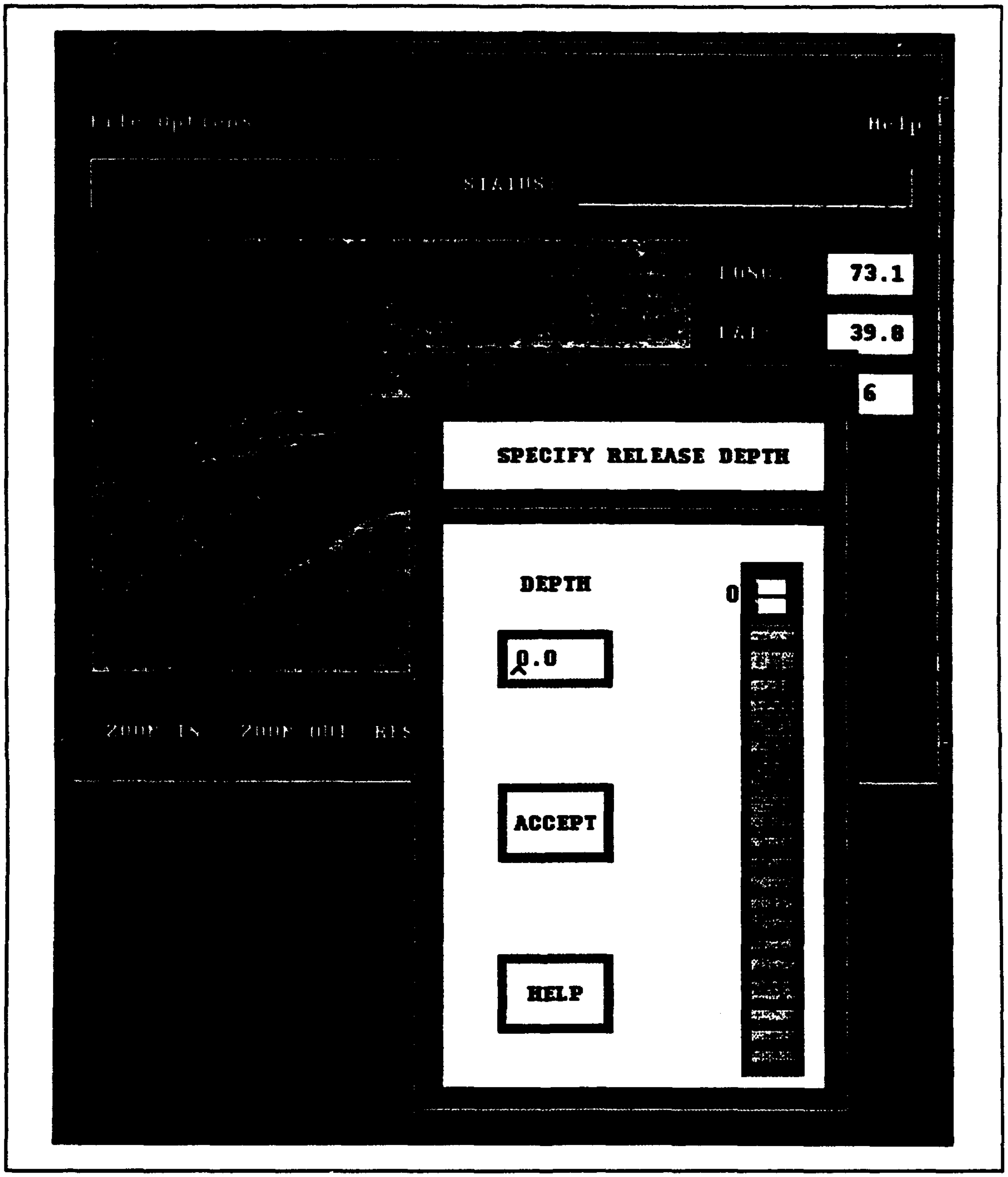

Figure 2. Release site specification screen

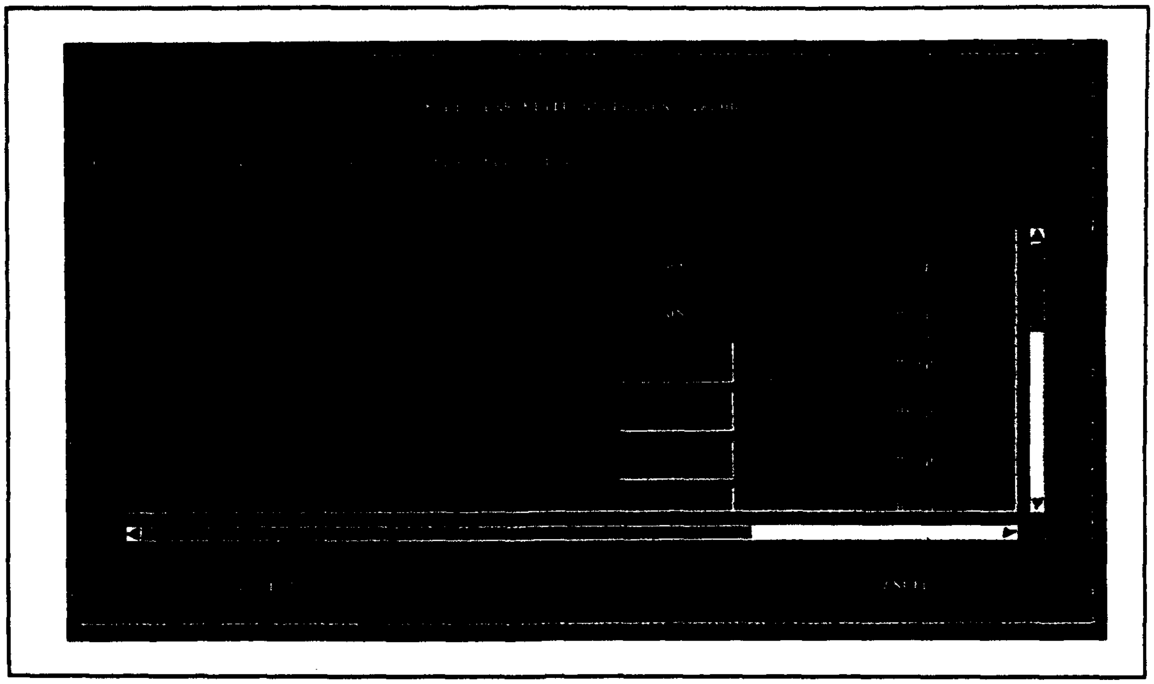

Figure 3. Model parameter specification screen

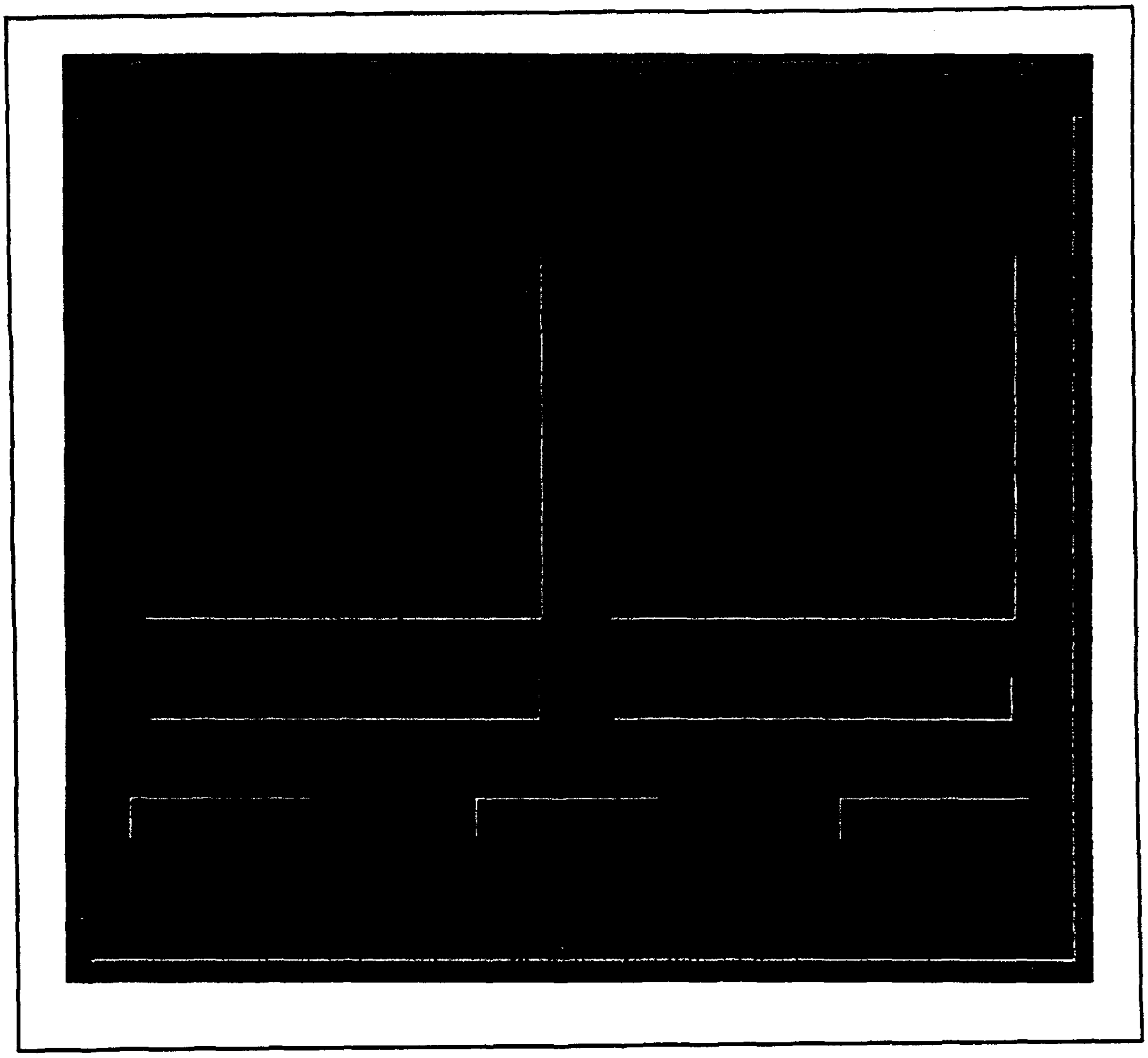

Figure 4. Model execution control screen

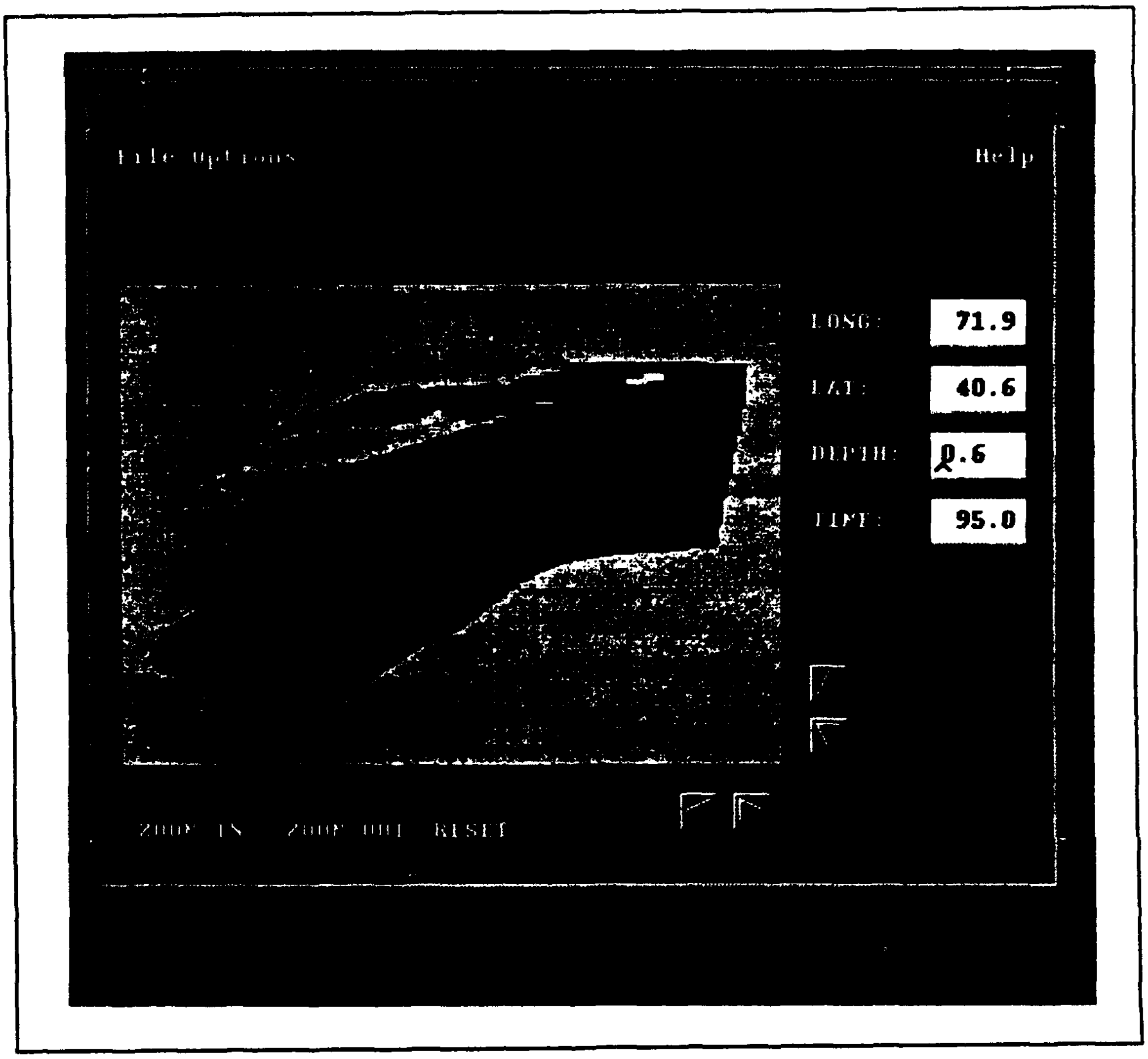

Figure 5. Model output display screen

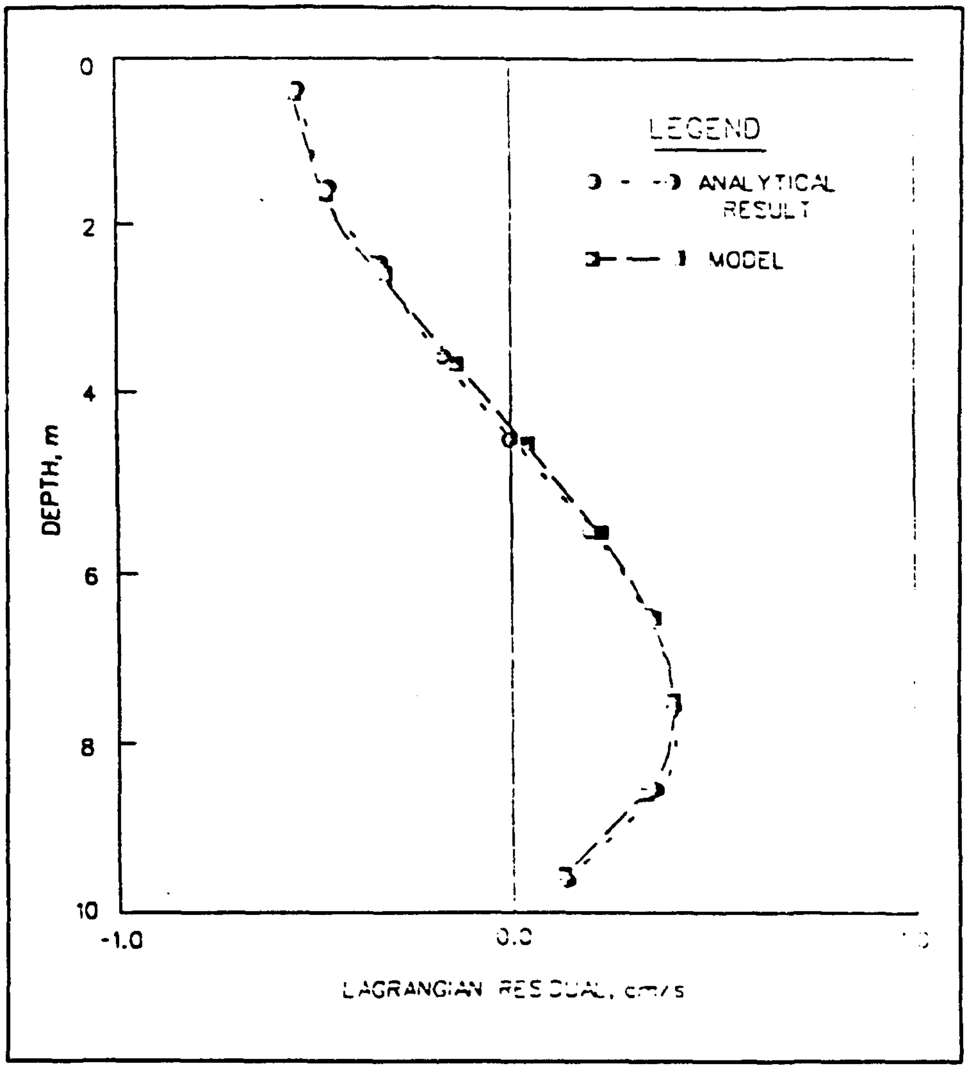

Figure 6. Comparison of predicted and analytical Lagrangian velocities

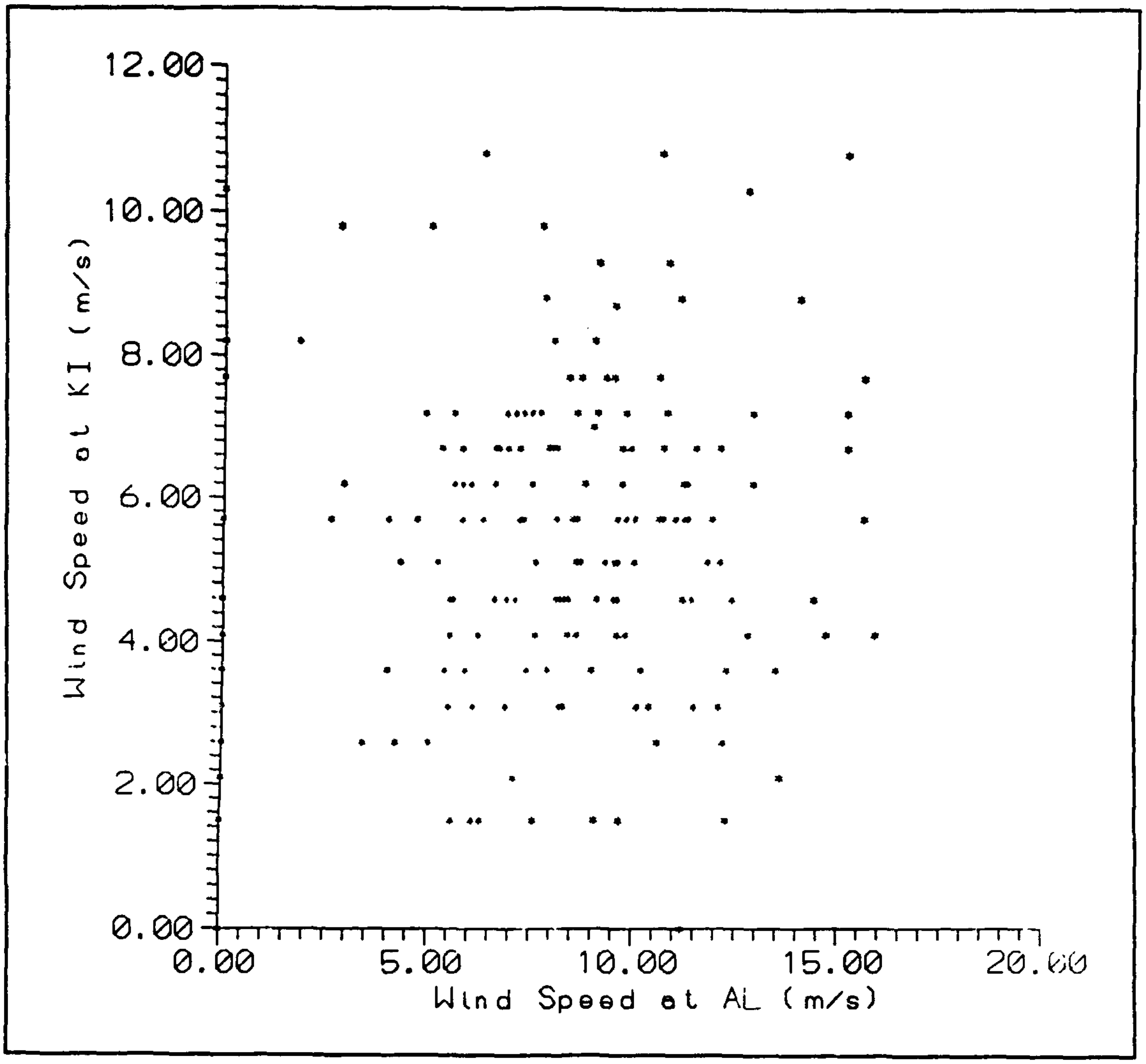

Figure 7. Wind speed comparison between Ambrose Light and Kennedy International

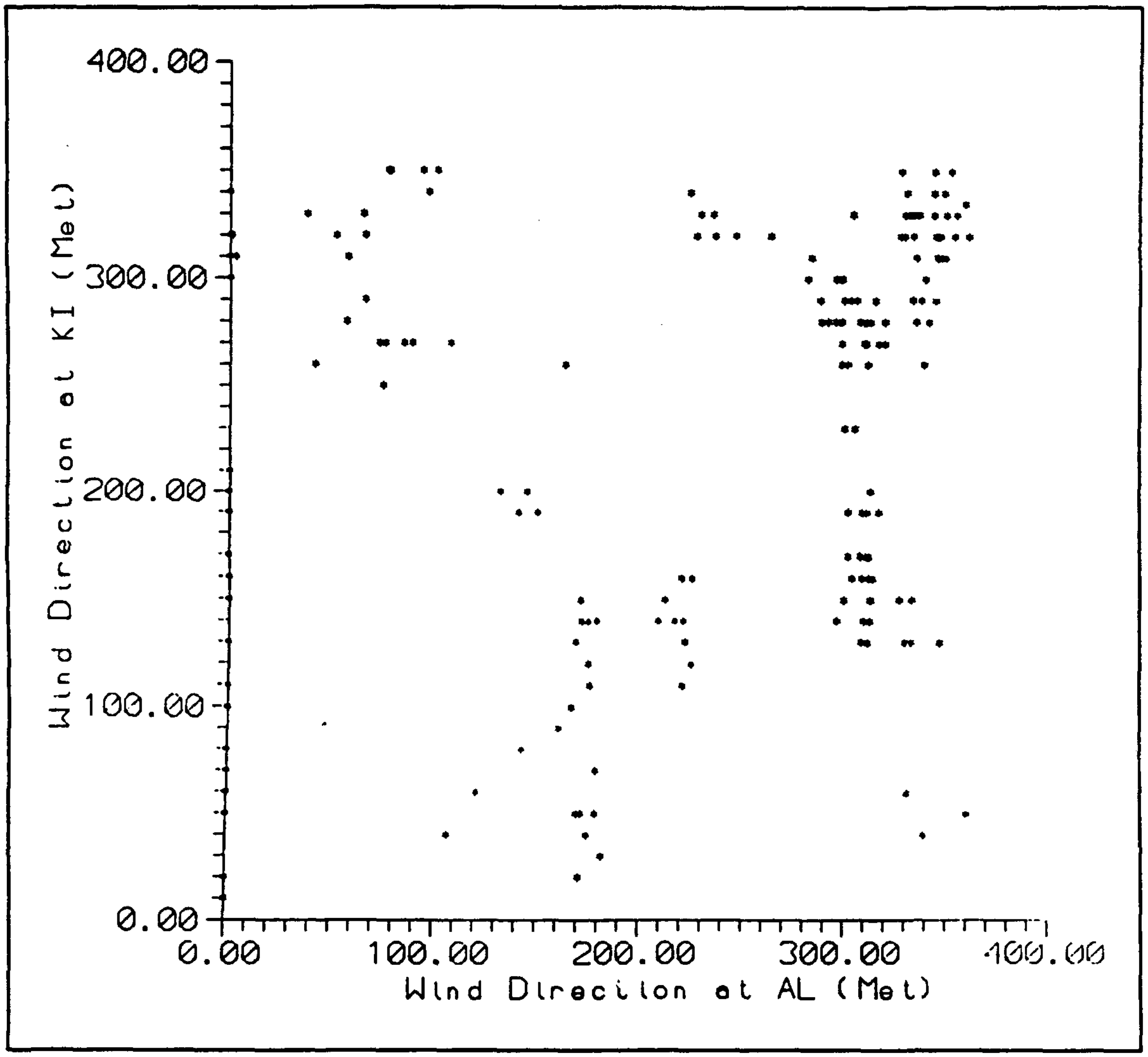

Figure 8. Wind direction comparison between Ambrose Light and Kennedy International (degrees from north)

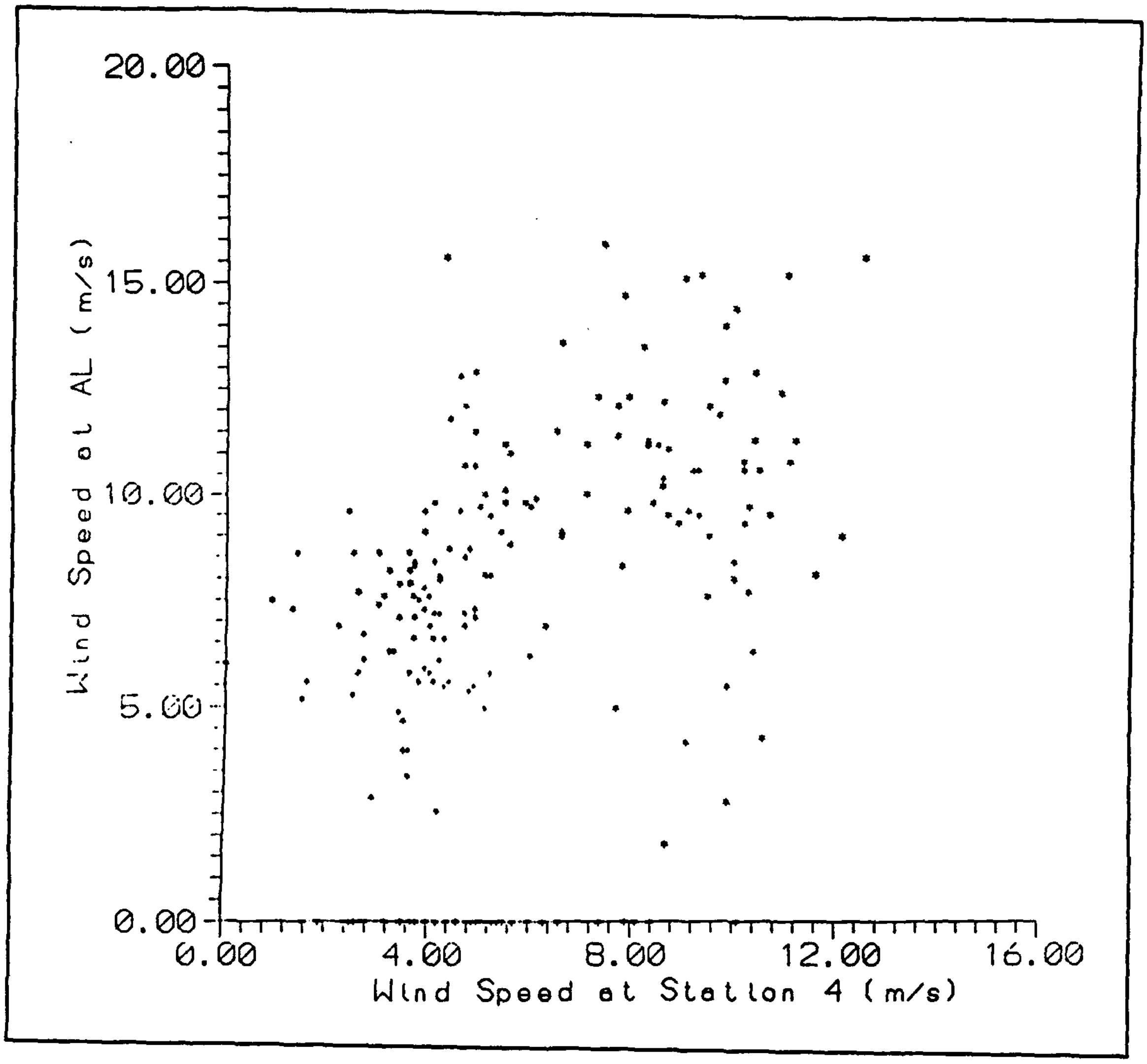

Figure 9. Wind speed comparison between NOAA Station 4 and Ambrose Light

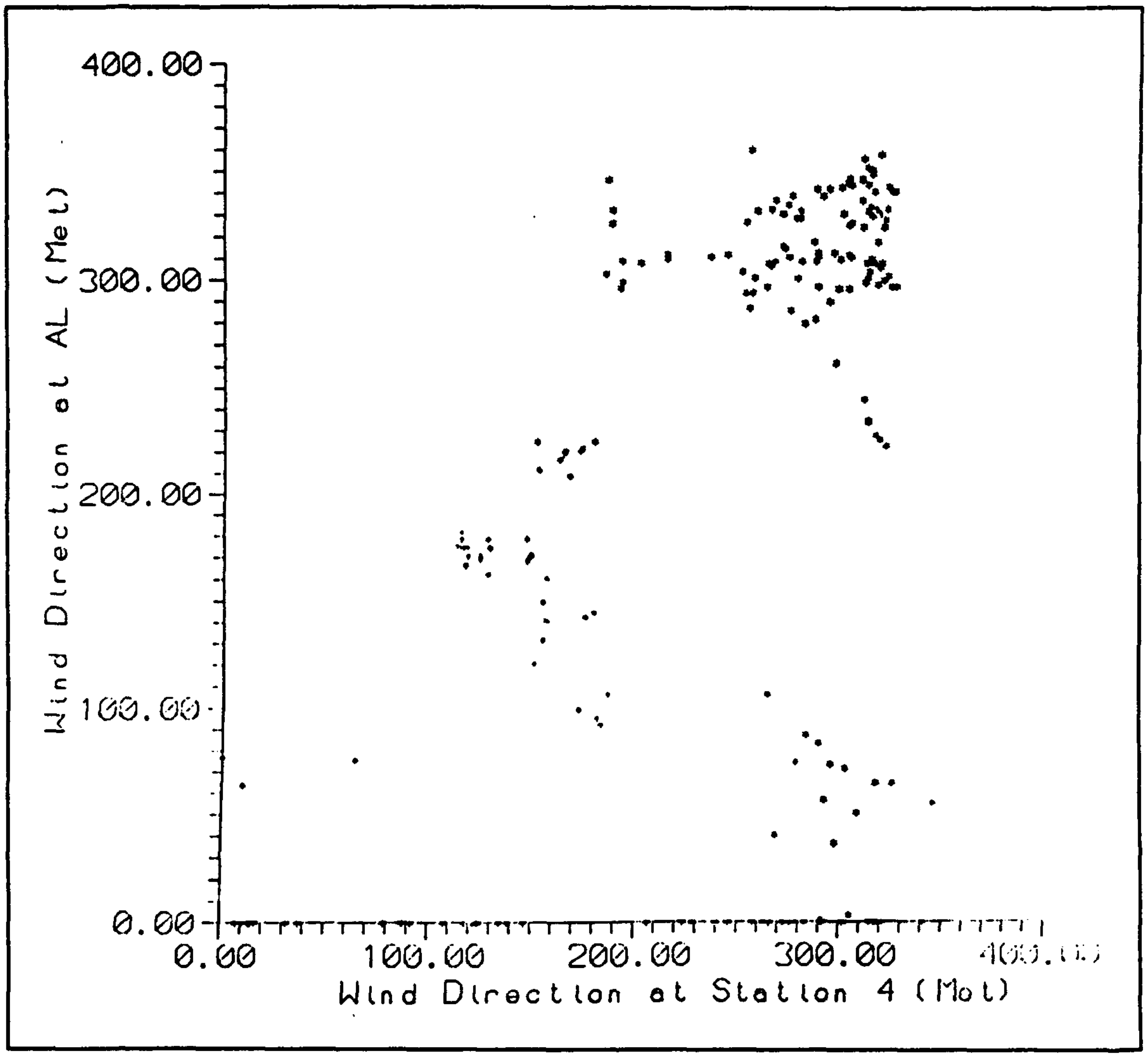

Figure 10. Wind direction comparison between NOAA Station 4 and Ambrose Light (degrees from north)

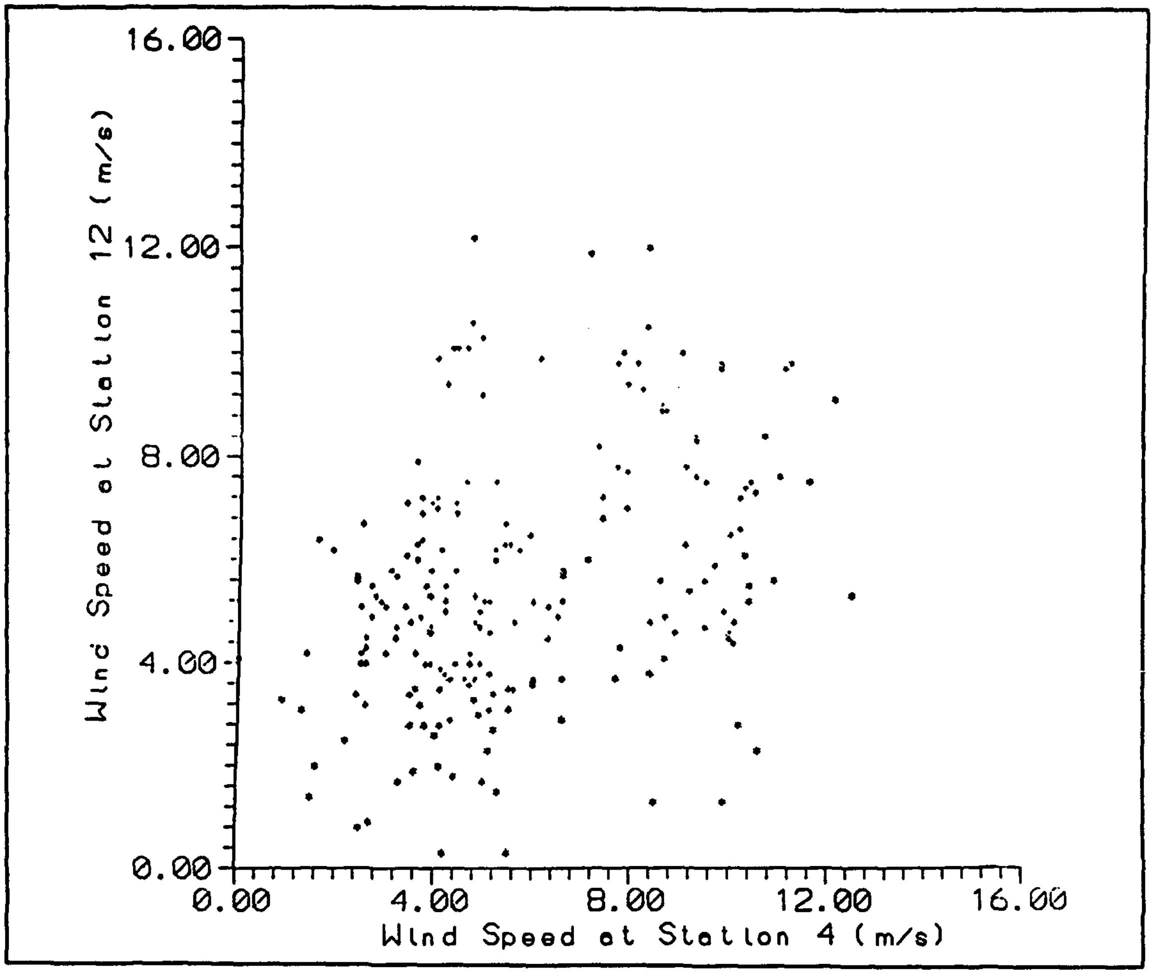

Figure 11. Wind speed comparison between NOAA Stations 4 and 12

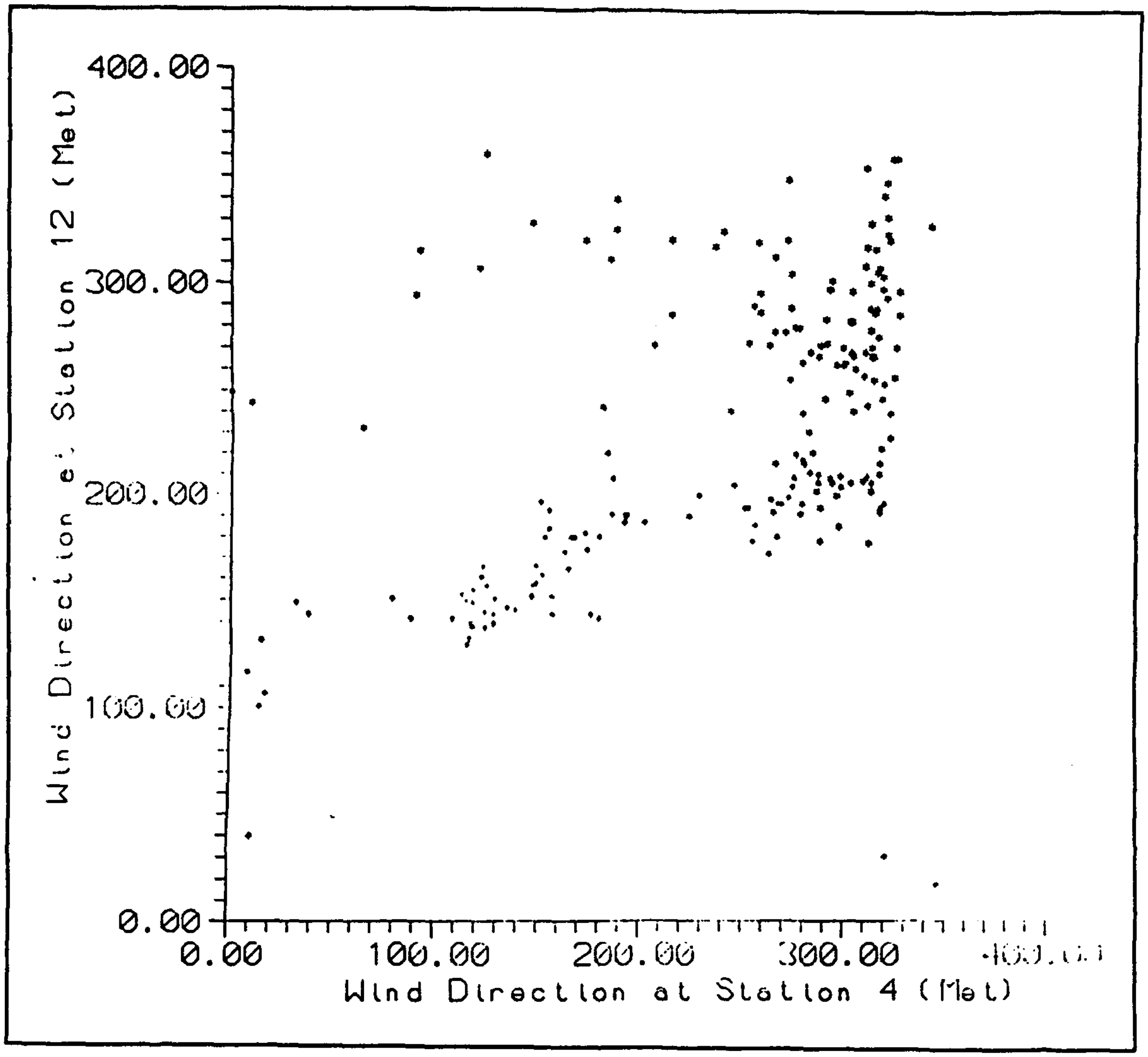

Figure 12. Wind direction comparison between NOAA Stations 4 and 12 (degrees from north)

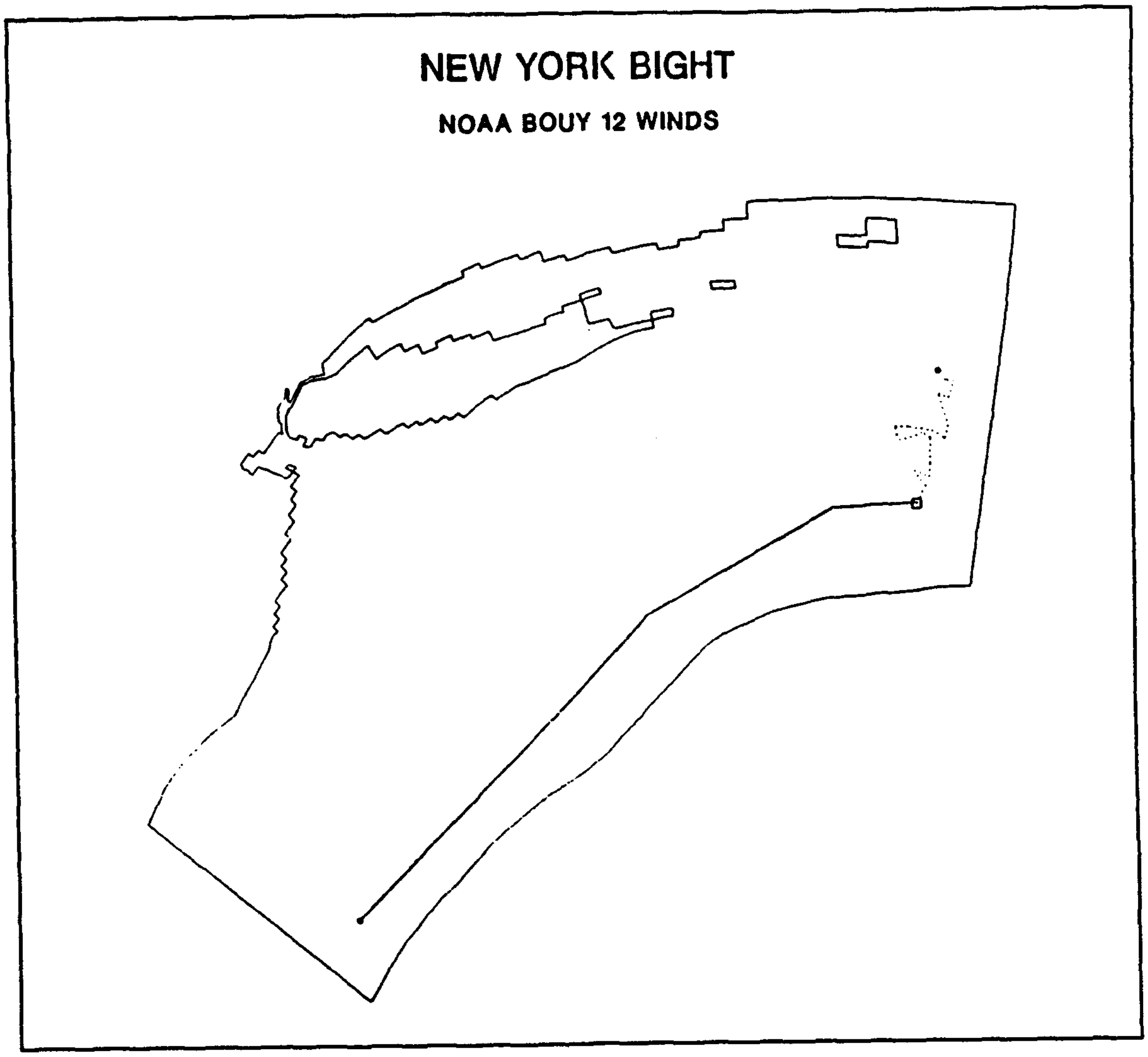

Figure 13. Predicted and observed drogue trajectories (.......predicted, ________ observed)

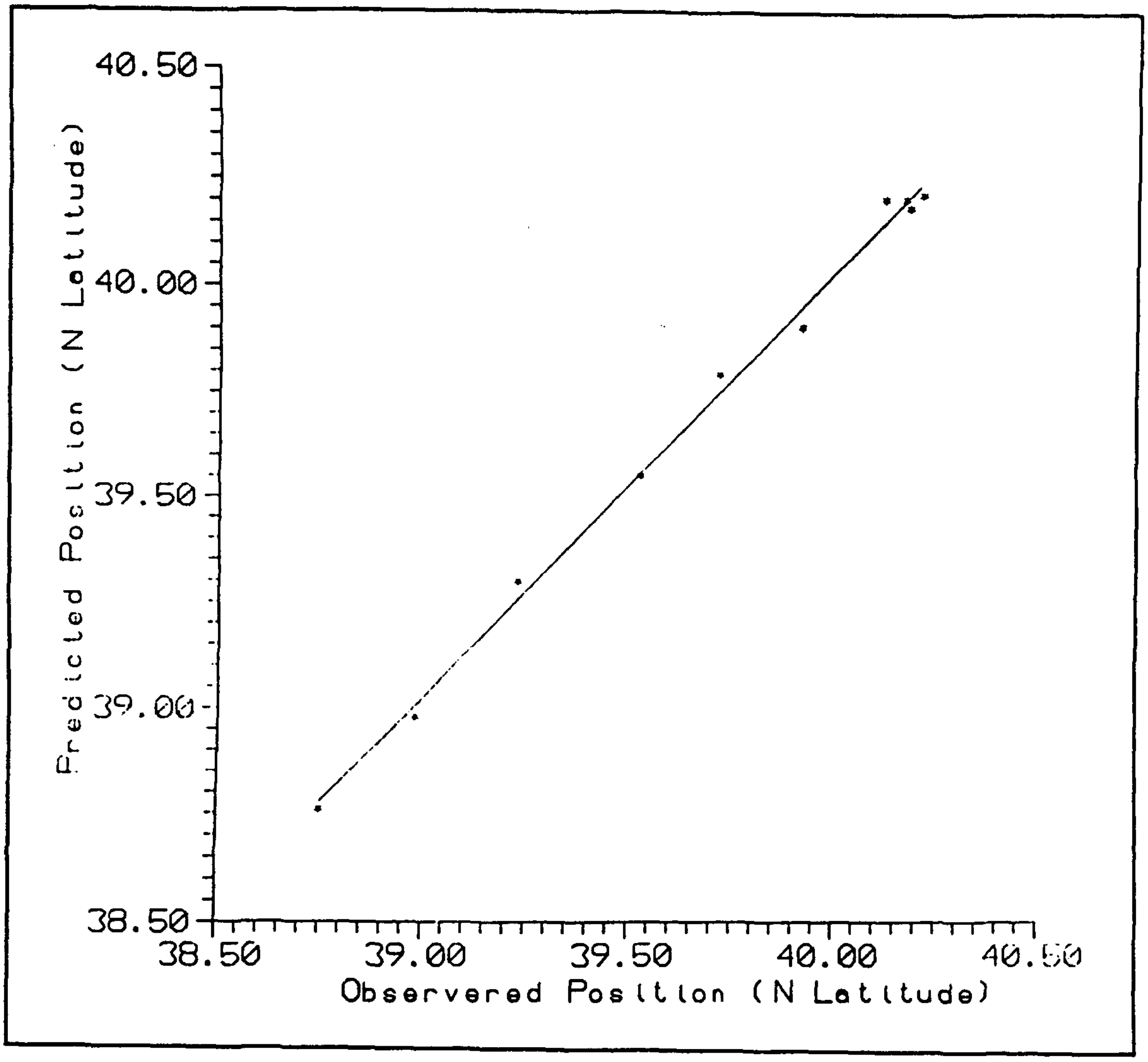

Figure 14. Predicted and observed drogue positions, latitude

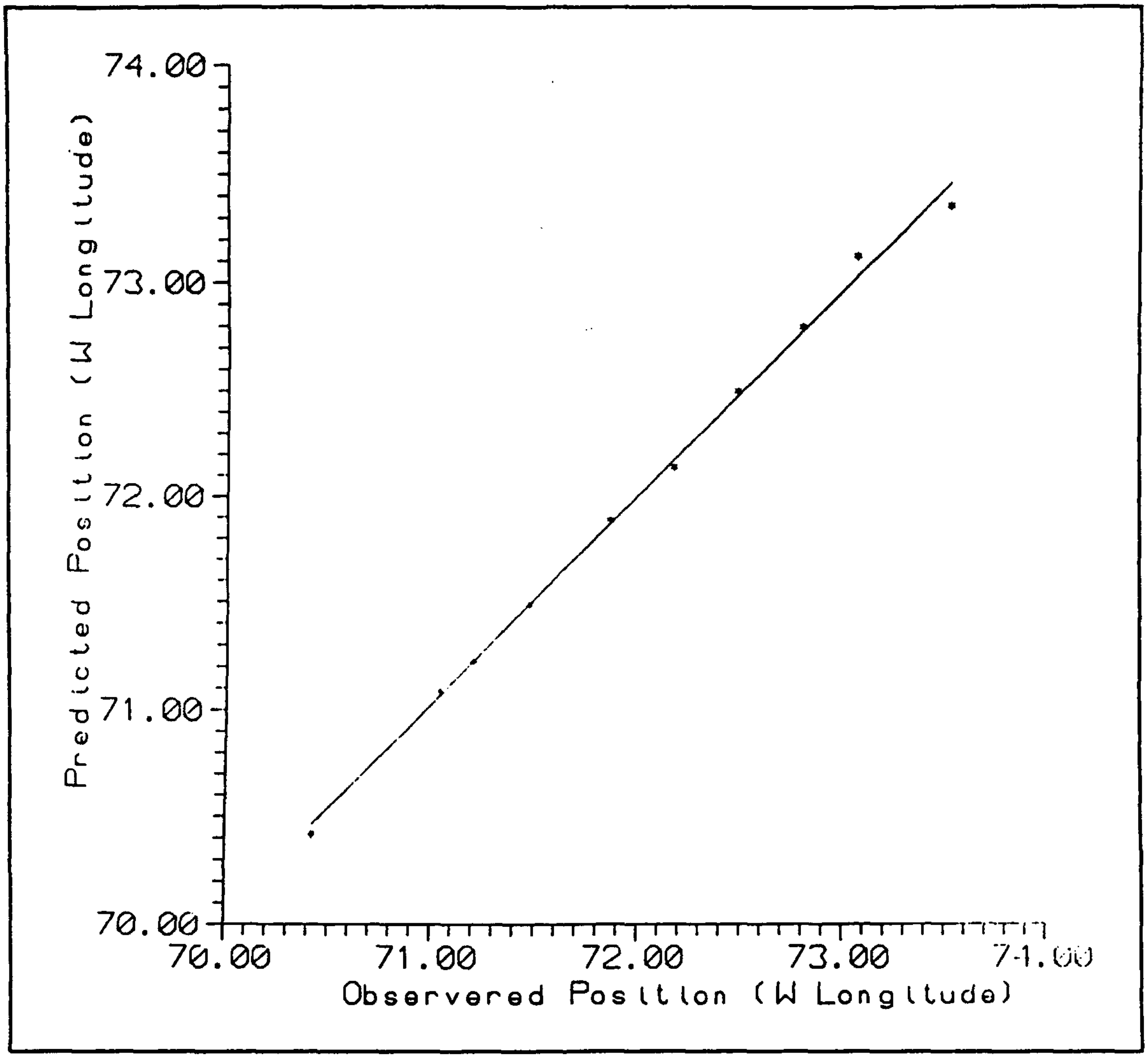

Figure 15. Predicted and observed drogue positions, longitude

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13. ABSTRACT *(Maximum 200 words)*

A three-dimensional particle tracking methodology for the New York Bight has been developed. Specific features included in the particle tracking model are surface transport of floatables by the wind and three-dimensional advection and diffusion of suspended and dissolved matter. The particle tracking model is run in conjunction with the Coastal Engineering Research Center's three-dimensional hydrodynamic model CH3D. The particle tracking model can be run in concert with CH3D as a series of subroutines or can be run in a stand-alone mode utilizing processed CH3D hydrodynamics. Interactive window-based software has been developed to assist in the setup and execution of the stand-alone particle tracking model.

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