Particle Tracking Model (PTM) in the SMS: I. Graphical Interface

PURPOSE: This Dredging Operations and Environmental Research (DOER) Technical Note (TN) describes the graphical interface for the Particle Tracking Model (PTM). The Coastal Inlets Research Program (CIRP) and the DOER Program are jointly developing the PTM. The PTM is described in a series of three technical notes. This technical note, Part I, describes the graphical user interface of Version 1.0 of PTM. Part II (Demirbilek et al. 2005a) provides an overview of general features and capabilities of PTM. Part III (Demirbilek et al. 2005b) is a tutorial with examples. The PTM has been developed for application to dredging and coastal projects, including dredged material dispersion and fate, sediment pathway and fate, and constituent transport. A technical report (MacDonald and Davies, in preparation) provides details about the theory and implementation aspects of the PTM.

INTRODUCTION: PTM methodology is based on a parcel calculation technique, in which parcels represent a given mass of sediment subjected to the same forces and exhibiting the same kinematics as a single sediment particle. Each parcel has its own set of attributes (e.g., grain diameter, specific gravity), which influence parcel behavior (entrainment, transport, settling). The PTM employs a Lagrangian particle tracking technique to estimate migration of sediment particles as influenced by the hydrodynamic forcing inputs, including current velocity and wave fields. This approach compliments the Eulerian sediment transport and morphological models, and can provide information about a specified subset of sediment processes. This information may be applied in projects without the more resource-intensive application of a Eularian sediment transport model.

PTM inputs are unstructured grid bathymetry, and time series of both water surface elevation, current velocity fields, and waves at each point in the modeling domain. The grid bathymetry is read from the standard IMS-ADCIRC (ADvanced CIRCulation model; see Luettich et al. (1992)) mesh file. The water surface elevation and current velocity fields are read from files written using the Generic Model Data Format standard (XMDF; see Jones et al. (2004)). Optionally, PTM also supports wave model or field data at grid points from a separate (Cartesian) grid. Wave input files to PTM are the standard STWAVE (Steady-state WAVE transformation model) output files (Smith et al. 2001). In addition to the hydrodynamic and wave input, the user specifies sediment sources, sediment properties, and model parameters to run PTM. The SMS interface of the PTM includes commands for layout of the model inputs including sediment sources, specification of the numerical parameters, and management of the Eulerian data (grids and solutions of ADCIRC and STWAVE). Both hydrodynamic and wave inputs are mapped to the PTM-specific computational grid. The velocity and wave fields must be computed or approximated (if desired) prior to constructing a PTM simulation in SMS. Result files for these fields are then used as input to a PTM simulation.

PTM I/O FILES: PTM requires five input files (Figure 1). These are the model parameters file (*.pcf), the particle source file (*.source), the native sediments file (*.sediments), the ADCIRC Eulerian grid file (*.grd or *.14), and the flow data in XMDF format (*.h5). Two other optional file types containing wave data and particle trap definitions may also be specified. The model may be launched from inside SMS, in which case the parameter file can be built through interface prompts. All other input file names and their locations are specified in the *.pcf file, along with the names and locations of model output files. Alternatively, the model can also be run outside of SMS using the parameter file as a command line argument. In this case, all input files must already exist.
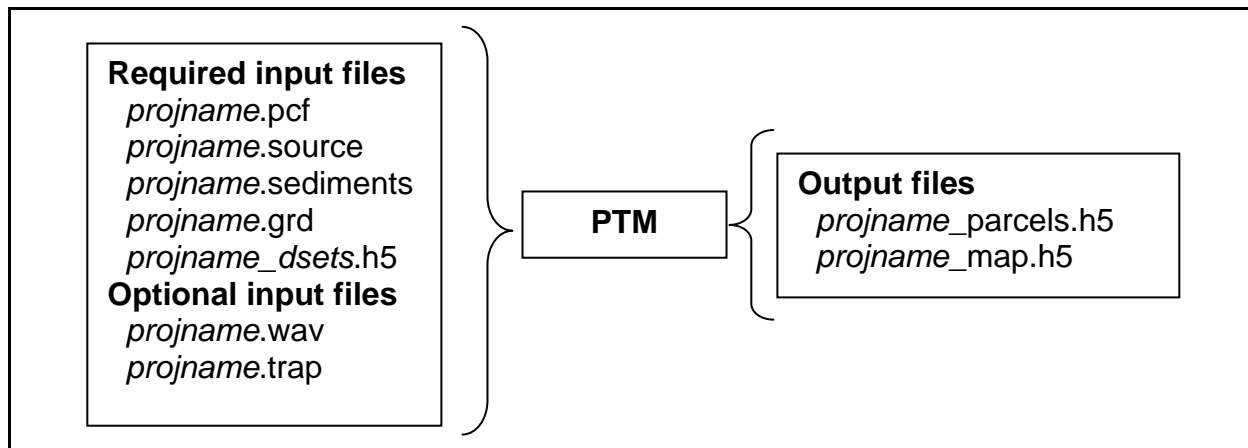
Required input files
  projname.pcf
  projname.source
  projname.sediments
  projname.grd
  projname_dsets.h5
Optional input files
  projname.wav
  projname.trap

PTM

Output files
  *projname*_parcels.h5
  *projname*_map.h5

Figure 1. Files involved in a PTM simulation

The model creates two types of output files, the particle and Eulerian mapped output files. The particle output file (*_parcels.h5) contains the paths and locations of individual parcels at each output time, along with attributes of those parcels such as their characteristic size, speed, source, and index. Parcel attributes that may be saved are briefly described in Table 1. Eulerian mapped data are output to the *_map.h5 file at each grid location. The Eulerian output includes wave parameters, flow values, bedforms, and computed mobility.

Table 1		
Particle Attributes Resulting from PTM Simulation		
Attribute	**Type**	**Description**
Grain size	Static – floating point	Size of a characteristic particle
Mobility	Transient – floating point	Tendency of the particle to move
Elevation	Transient – floating point	Elevation of the particle above the sediment bed
State	Transient – integer	=0 for dormant particle, =1 for moving particle
ID	Static – integer	Particle ID
Source	Static – integer	Particle source identifier
Parcel mass	Static – floating point	The total mass of particle

The PTM output files are in binary format, and written as hdf5 files in XMDF standard (http://www.wes.army.mil/ITL/XMDF). These files allow for storing large simulations in a compressed form to speed up data processing and viewing, and ensuring portability of the

compressed data across different computing platforms. The binary file format also allows users to run the PTM on one computing platform and perform post-processing on a different computing platform. The default computing platform for the PTM simulations is a PC, and all of these tasks can be performed on a PC.

PTM INTERFACE: The PTM interface in SMS is accessed through the *Particle Module* 🔀 of SMS. User assistance for SMS is available through the "Help" icon within SMS and the SMS users guide (Zundel 2005). A general description of the interface follows. A simulation can be initiated by choosing the *New Simulation* command in the PTM menu, or by opening an existing simulation using either an *SMS* project (.spr) file or a PTM program control file (.pcf). The PTM uses the *Map Module* 🧭 to define the source terms for particles, and may use the *Mesh Module* 🔷 to visualize, select, and possibly convert the current data. PTM also utilizes the *Cartesian Grid Module* ⊞ to convert, visualize, and select wave input data.

The PTM interface primarily consists of the PTM menu and various sub-menus in the *Particle Module*, and the PTM coverage in the *Map Module*. The *Particle Module* is used to specify user input and create the *.pcf file and the *Map Module* is used to define the particle source terms. This document describes the standard components of the PTM interface. It is recommended that the user become familiar with other modules of SMS to fully exploit the many intricacies and features of the PTM interface.

PTM menu. The PTM menu and commands are listed and described in Figure 2 and Table 2, respectively.
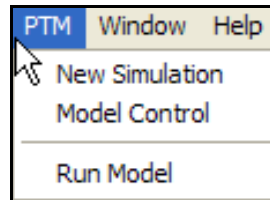

Figure 2. PTM Menu

Table 2 PTM Menu Commands	
Command	**Functionality**
New Simulation	Creates a new PTM simulation. A simulation includes a set of particle sources, sediment conditions, run parameters, and the corresponding particle paths computed by PTM once the model has been executed.
Model Control	Brings up the Model Control dialog to specify model simulation parameters for the present simulation.
Run Model	Brings up a dialog to allow users to select the executable of PTM to run with the present simulation. As the model runs, a dialog monitors progress of the model and gives the user status messages. After the run is complete, the spatial solutions are read in for analysis and visualization.

Specifying simulation parameters. The PTM simulation dialogue stores all the model parameters and input files used in a simulation. To specify these parameters the user selects the *Model Control* command from the PTM menu, which invokes the PTM *Model Control Dialog*. This dialogue consists of six separate pages (Figure 3-9), discussed below:

- *Computational parameters dialog page* (Figure 3). This page allows the user to select computational methods and parameters from the available list of capabilities. Computational methods include choosing whether particles will be distributed by weight or by grain size, whether Eulerian interpolation will use the van Rijn (1984 and 1993) or PTM method, whether the particle centroid will be computed by the Rouse (1939) or van Rijn method and whether advection will use the 2D or quasi-3D method. User-specified computational parameters in the Model Control dialogue box include the specification of a minimum cut-off depth, water temperature, salinity, transport factor, and diffusion parameters. The minimum cut-off depth refers to the minimum water depth for which a particle will be tracked. The minimum depth is used to limit calculations at near-zero depths; typically this is set to 0.01 m, but may need to be set lower if working on very fine scale or laboratory problems. If a particle moves into a region of the domain with a water depth lower than the cutoff depth, the particle is considered inactive until water level rises enough to increase the depth above the cutoff depth. The user also specifies how often the shear, bedforms, and mobility should be recomputed. The user is referred to the technical report (MacDonald and Davies, in preparation) for a description of these methods and appropriate application.

- *Hydrodynamic, sediment, and source input dialog page* (Figure 4). This page is used to specify input files for bathymetry, flow (current and water surface elevation), and native sediment parameters. This box is also used to define particle sources. As noted above, the model requires a Eulerian grid to define the bathymetry, native sediments, water surface, and the velocity field. If these files exist in the appropriate format, they can be accessed directly without loading the grid
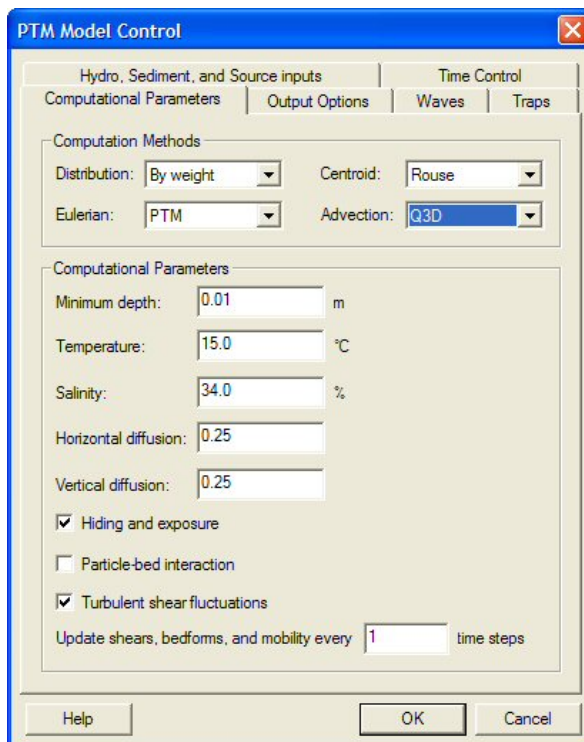

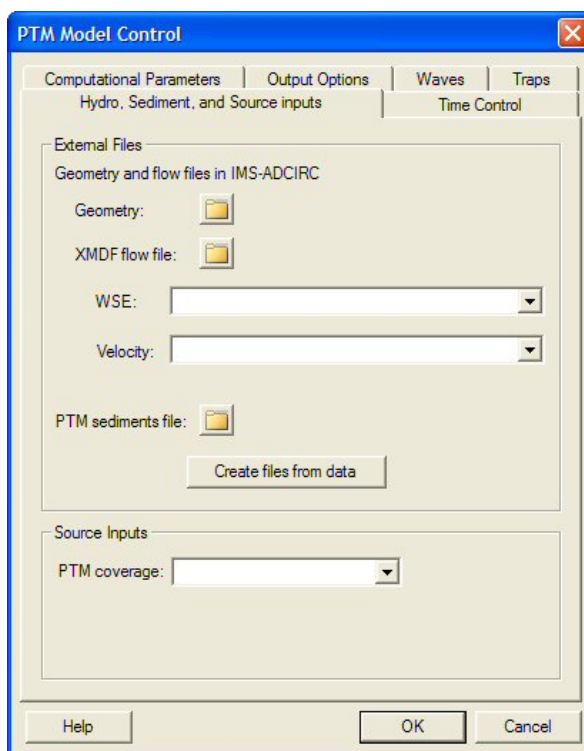Figure 3. Computational parameters page of PTM Model Control Dialog

Figure 4. Hydrodynamic, sediment, and source inputs page of PTM Model Control Dialog

4

into SMS. If the files do not exist in the appropriate format, SMS can be used to convert existing Eulerian data to the correct format using the *Create Files from Data* button. This button displays the *Create PTM external input files* dialog (Figure 5).

The top section of this dialog is used to select the Eulerian grid geometry file. Clicking on the *Choose* button displays a list of the Eulerian objects that have been loaded into SMS. This could be a finite element mesh, or a curvilinear grid, or a scattered triangular mesh from hydrodynamic models. The only limitation is that the object must have bathymetric, water surface, and current data defined in a data set for each computation node in the grid. These data will be converted to the appropriate PTM structure within the SMS interface. The PTM solution/ output time units are also specified in the interface. The SMS converts from days, hours, or minutes into seconds as required for PTM calculations. As shown in the top part of the panel (Figure 5), the PTM reads in ADCIRC-format fort.14 file and creates a PTM geometry file in the same format. In the flow files section of the dialog, the user may select ADCIRC-format for current and water elevation files to be saved as PTM input files. The SMS creates the PTM input files when the user clicks the *OK* button. The bottom
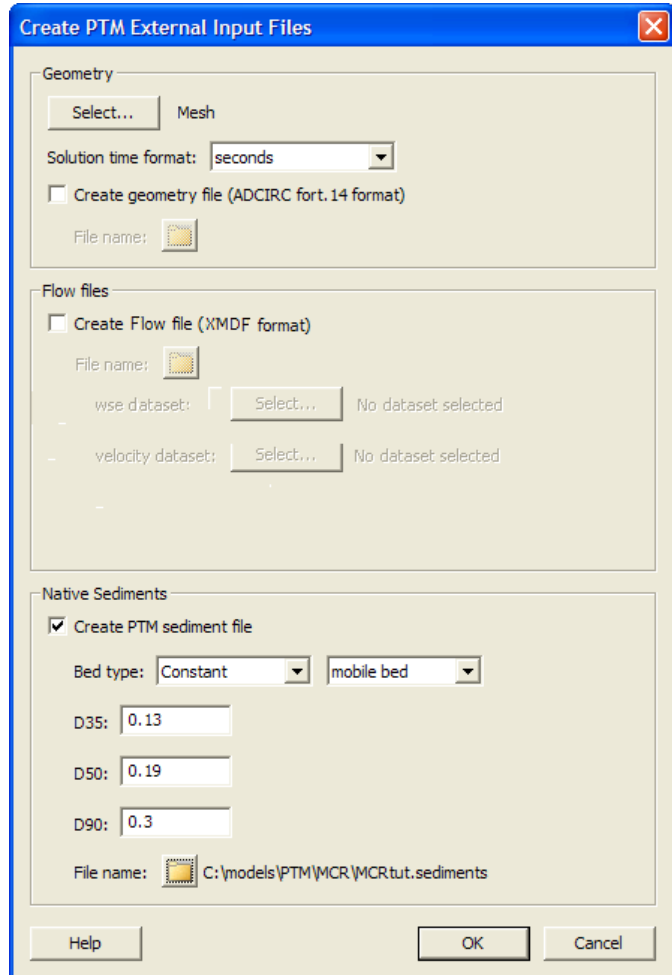

Figure 5.   Dialog to create input files from Eulerian grid in SMS

panel allows the user to create the native sediments file. This file includes the characteristic grain sizes (in millimeters) of the native bed. A negative value of d_{90} indicates a hard-bottom bed and the value supplied would represent the roughness factor (millimeters). Native sediments are not resuspended in the PTM because they are not a particle source, but they are used to compute roughness, bed forms, and active layer mixing, thereby affecting turbulence and particle mobility.

- *Time control dialog page* (Figure 6). The time control page of the PTM Model Control dialog is used to specify simulation dates and the time-step size. Input parameters are: start date/time, end date/time, computation time-step, output interval, and hydrodynamics start time. The hydrodynamic solution must start at or before the starting PTM simulation date/time, and must contain valid data for the entire PTM simulation period. Guidance for selecting the simulation time-step is provided in the PTM technical report (MacDonald and Davies, in preparation). In

another dialog box, the user specifies time periods of the particle sources. These time periods must be included in the computational time range defined in the Time Control dialog.

- *Output control dialog page* (Figure 7). The *Output Options* page allows the user to specify which model results to save to the output files during the PTM simulation. PTM creates two solution files. One stores the particle data (Lagrangian), and the other stores the mapped Eulerian data. They are named by adding on to the simulation name. The top portion of the page defines which particle-related data sets are saved to the "*SimulationName_*particles.h5" file. The bottom portion of this dialogue allows the user to select data to be mapped back to the Eulerian grid and saved to the "*SimulationName_*maps.h5" file. The user also specifies how often each data type should be saved.

- *Wave input dialog page* (Figure 8). This page is similar to the hydrodynamic, sediment, and source inputs page described previously. It allows the user to specify a wave field input file for the PTM simulation. The user specifies the origin and orientation of the grid. If the grid is loaded into SMS, the "*From STWAVE Grid*" button will fill in the origin and angle based upon the grid. In the lower portion of the dialog, the user can input output file name (*.wav) and time stamp for the wave input file.

- *Trap control dialog page* (Figure 9). The *trap control* page allows the user to specify the timing control of the polygonal traps defined in the PTM coverage. The user can also specify whether the traps will retain the particles as they arrive, and if they do not retain them, whether to count particles that enter the trap multiple times as a single instance or multiple instances. The PTM technical report provides more detail on using traps in PTM simulations.
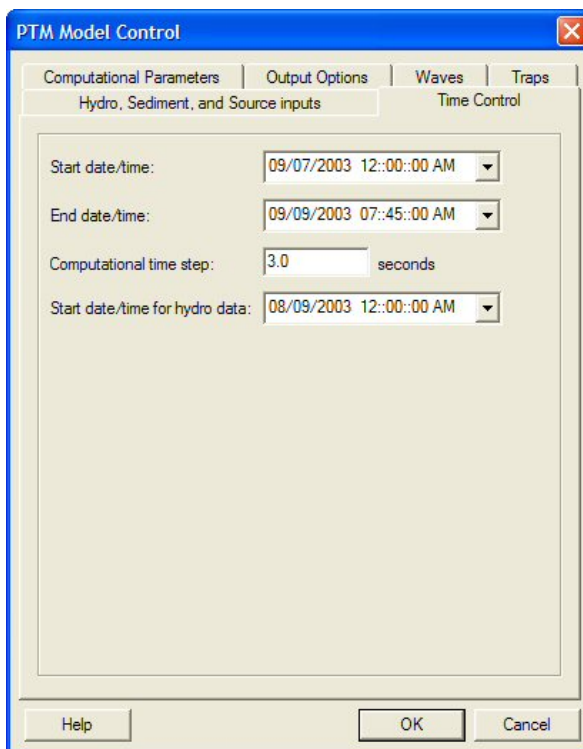

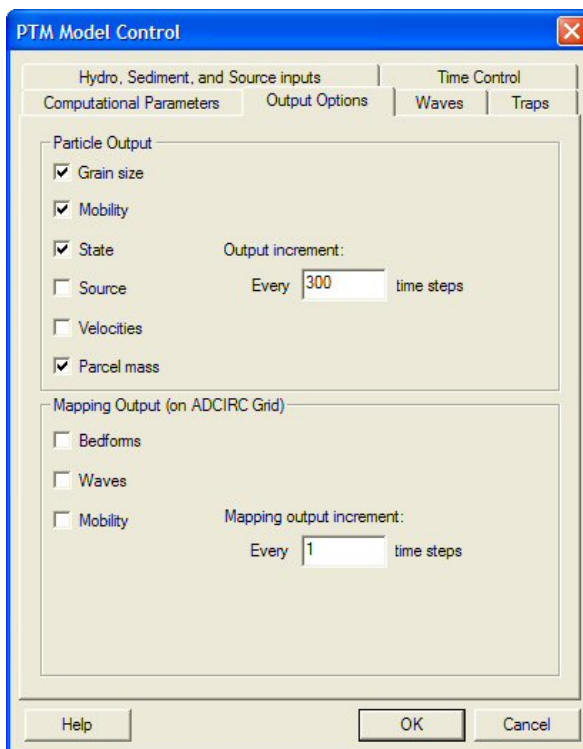Figure 6. Time Control page of PTM model control dialog

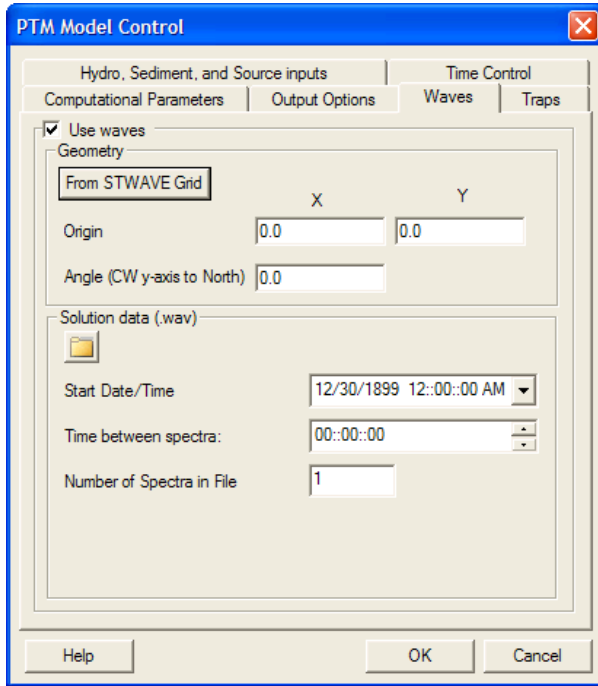Figure 7. Output control page of PTM model control dialog

6

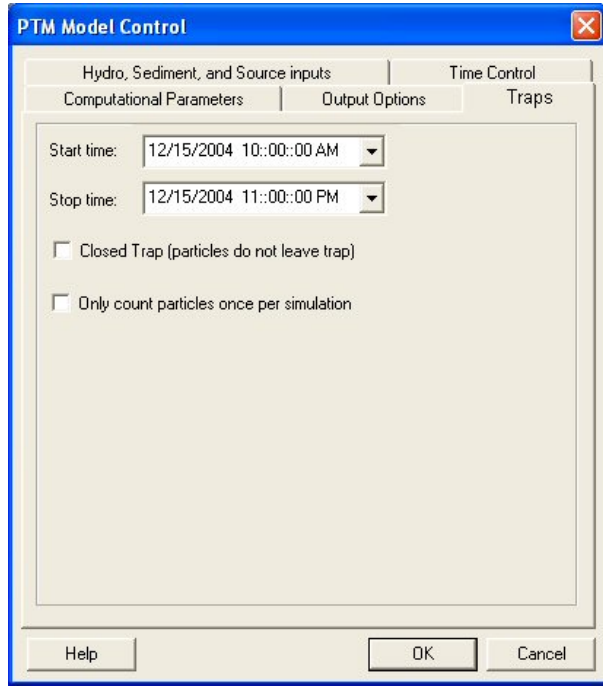Figure 8.   Wave control page of PTM model control dialog

Figure 9.   Trap control page of the PTM model control dialog

Specifying particle sources. Particle sources are defined as attributes on nodes and arcs (Zundel et al. 1998; Zundel 2005) in the PTM coverage in the *Map Module* , i.e., PTM sediment sources are defined at a point or along a path. The positions and attributes of each time-varying source are managed in the map module of SMS through the *Feature Objects/Attributes* command. The source attributes can be managed and edited using the Feature Attributes command in the map module. The user can create feature points in the map module, and by double-clicking, assign attributes to any feature point to define it as a particle source. Figures 10-13 illustrate the SMS-generated dialogs (tables) for each of the source types. Each row of the table represents a point in time describing the life of the source. For times between rows, each column of data is linearly interpolated from the rows before and after it. The first column of the table includes the date and time. The table also includes a central position (x,y) for the generation of particles, elevation, and characteristic size. The position of each particle generated actually varies across a specified radius (both horizontal and vertical). Further, the size of the characteristic grain of the particle varies according to a specified grain size distribution, characterized by the standard deviation of the sediments. For details, see MacDonald and Davies (2005). Particle source types include:

- *Point source of certain mass rate* (Figure 10). A mass rate point source produces particles at a specified rate over time. Each row in the table defines the point source central location at the time specified in the first column. Point source locations between the times specified in any two adjacent rows are interpolated between the locations specified in each row. The generation rate, characteristic grain size, and other attributes also vary with time. This

7

method of particle release can be used, for example, to represent effluent loss from a pipeline that is moved intermittently.

Figure 10. Mass rate point source attribute table

- *Point source with instant mass* (Figure 11). An instant mass source creates an entire group of particles at specific points in time. The times are specified in the first column of each row and the remaining columns control the amount of mass, the mass in each particle, and the other particle attributes.   As with mass rate sources, the particle initial positions are distributed randomly around the central location to allow for a natural variability. This method of particle release can be used, for example, to represent release from a split-hull barge during dredged material placement.

Figure 11. Instant mass point source attribute table

- *Vertical line sources at a planar point* (Figure 12). Point sources may be used to represent a set of vertical line sources. At the top of the dialog, the user specifies the number of bins in the line source and the maximum height above the bottom that particles will be generated. To the right of this information, the user enters the rate of particle generation for each vertical segment as a percentage of the total mass of particles generated. The vertical line is segmented into equal increments (height divided by the number of bins). The table at the bottom again defines the timing of the particle generation (the first column), the central position of the particle generation (second and third columns), and the particle attributes as described above (columns 4-10). Particles are distributed linearly along the line and according to a Gaussian distribution around the line. This source can be used, for example, to simulate vertical distribution of sediment released into the water column from a moving dredge.
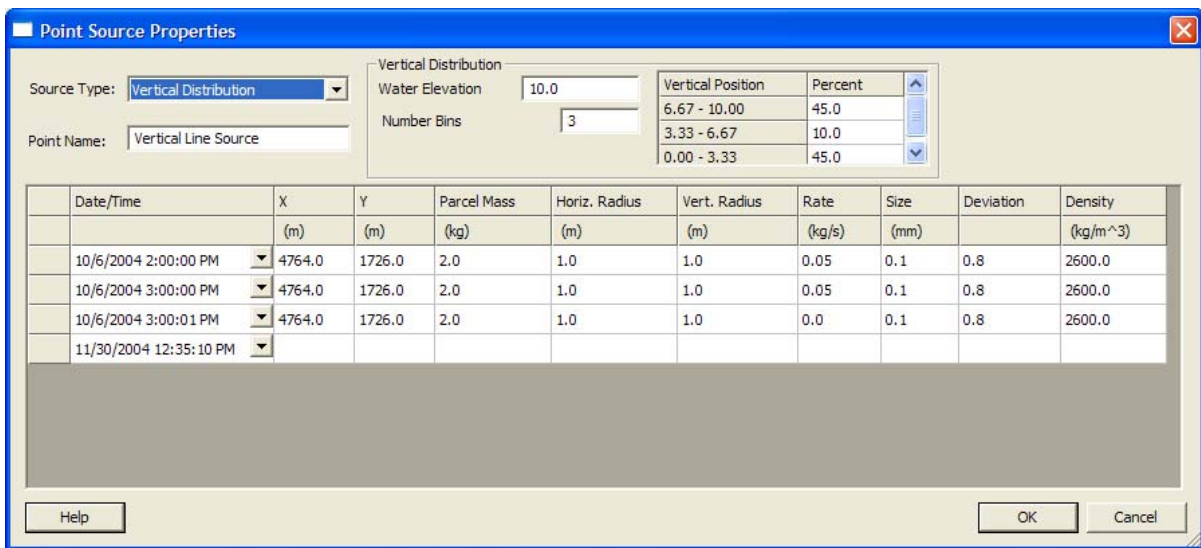
Date/Time	X	Y	Parcel Mass	Horiz. Radius	Vert. Radius	Rate	Size	Deviation	Density
	(m)	(m)	(kg)	(m)	(m)	(kg/s)	(mm)		(kg/m^3)
10/6/2004 2:00:00 PM	4764.0	1726.0	2.0	1.0	1.0	0.05	0.1	0.8	2600.0
10/6/2004 3:00:00 PM	4764.0	1726.0	2.0	1.0	1.0	0.05	0.1	0.8	2600.0
10/6/2004 3:00:01 PM	4764.0	1726.0	2.0	1.0	1.0	0.0	0.1	0.8	2600.0
11/30/2004 12:35:10 PM									

Source Type: Vertical Distribution
Point Name: Vertical Line Source

Vertical Distribution
Water Elevation 10.0
Number Bins 3

Vertical Position	Percent
6.67 - 10.00	45.0
3.33 - 6.67	10.0
0.00 - 3.33	45.0

Figure 12. Vertical line at a point source attribute table

- *Horizontal line source* (Figure 13). A horizontal line source is situated along a straight line with two end points having a constant elevation. Particles are generated evenly (uniformly) along this straight line. The line can move over time. Each row defines the position of the line at a particular time, which is specified in the first column. The positions of particles are defined in columns 2-7. The remaining columns define the particle attributes as defined above.

Figure 13. Horizontal line source attribute table

Visualizing PTM solutions. The principal output from PTM is a series of particle locations over time and attributes of those particles at each time (the *_particle.h5 file). The SMS includes tools for visualizing the particle paths. These tools reside in the *Particle Module* 🐾. The solution file is read into SMS using the File|Open command. Particle data sets and attributes appear under the name of the simulation in the *Project Explorer* dialog (tree window) in SMS (Zundel 2005) as shown in Figure 14. In this example, PTM output (see Figure14) consists of particle sources (which stay constant for all times), particle states (active or inactive, i.e., mobile or immobile), and particle velocities. The latter two change from one time-step to another. The user can select an active data set in the upper portion of the tree, and an active time-step to display in the lower portion of the tree.
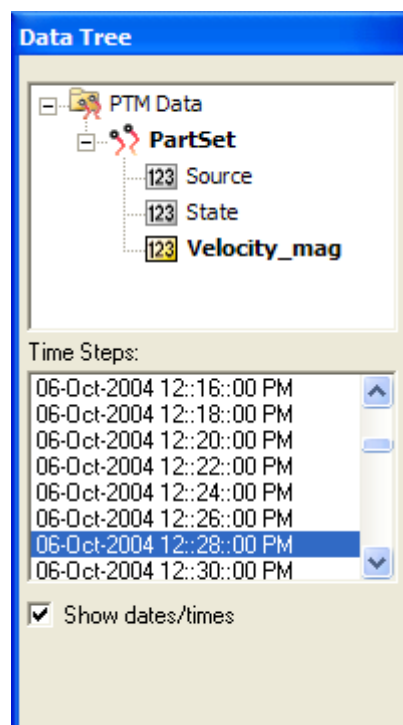

Figure 14. Particle data sets in the project browser and the time-steps

- *Particle display options (Figures 15 and 16).* The display options in the SMS interface allow users to specify which particles to display and how they should be displayed. Options include displaying the particle at a point in time, the particle path (over the whole particle life), and/or a portion of the path (specified as a time length). These options are depicted in Figures 15 and 16. The display options are shown in Figure 15. The three toggles allow the user to set the display status of the particles, the particle tails (portion of the particle path), and the particle paths. By clicking on the small buttons, the user can change the line thicknesses and colors, and set the symbol to be used for the particle. Particles and particle tails can be color coded to display their attributes by choosing to color particles based on the data sets read from the solution file. In the lower right side of the dialog, the user can choose to filter the number of particles to be displayed.
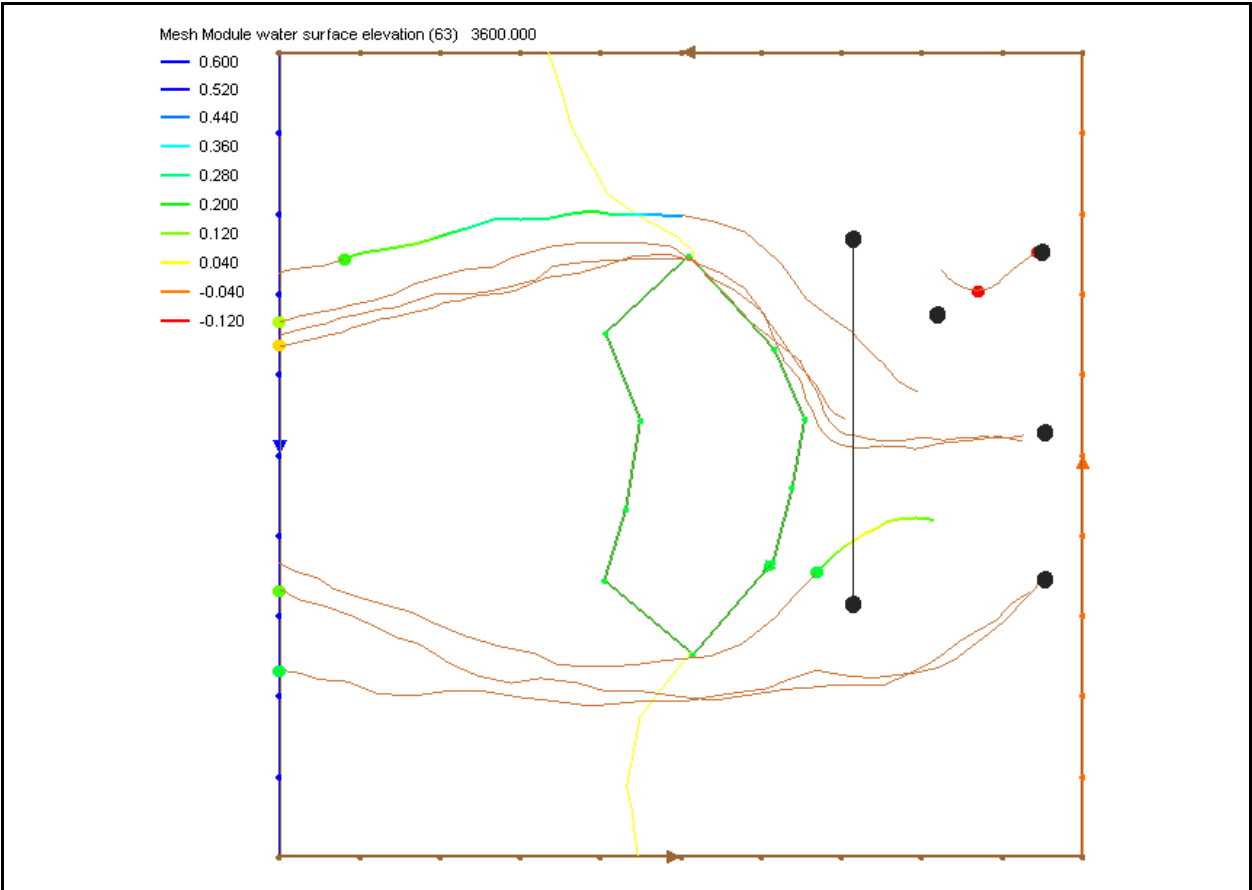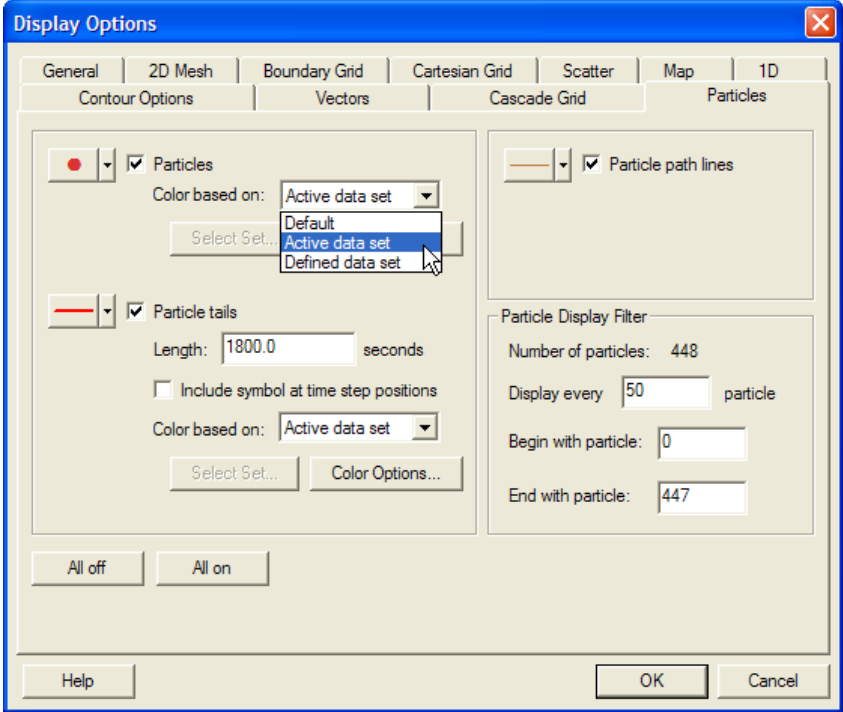
10

Figure 15. Particle module display options

Figure 16. Particle heads, paths, and tails

Figure 16 is an example display of PTM output. The particles and their tails are colored based on the velocity of the particle. The variation in path color demonstrates the change in velocity over the particle path, and the length of the tail shows how far the particle has traveled in the last half hour. The user specifies this value. The complete paths are shown as thinner, brown lines.

- *Particle selection.* The particle selection tool ⬚ can be used to select a specific particle or group of particles. If a single particle is selected, SMS displays the exact value from the current data set or attribute. In other words, if the particle velocity is selected in the Project Explorer, and a user selects a particle, the computed velocity for that particle is displayed. The tool also provides information about the number of particles in a specific area and the average value of the data set for the particles in that area.

- *Data menu.* Several tools that can assist with visualization are available through the SMS particle module data menu shown in Figure 17. These are:
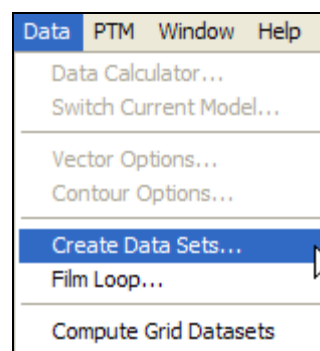
  o *Create data sets.* This command allows the user to generate additional data sets for each particle throughout the time range of the simulation. The particles and their tails can be colored based on the values in these data sets. Figure 18 illustrates the dialog provided to create these data sets. The user selects which data sets to create, and a name for the computed data set.
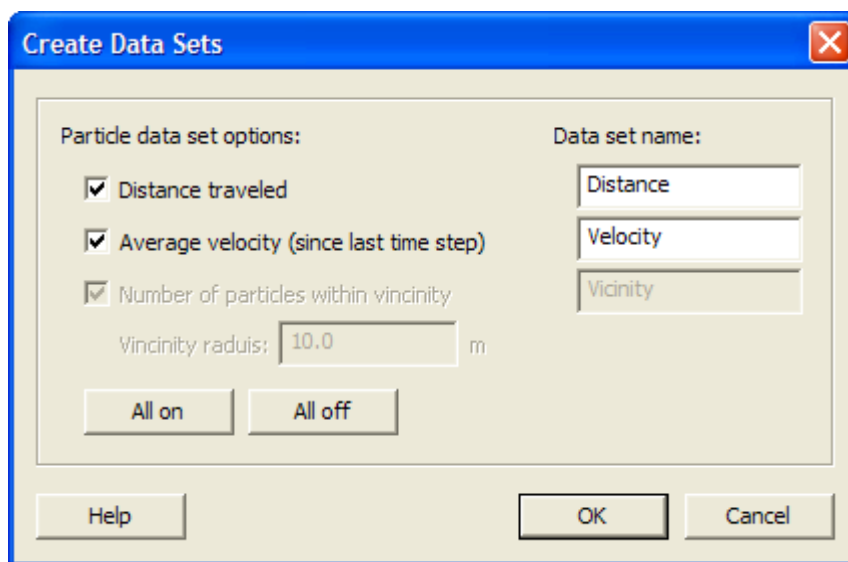
Figure 17. Particle data menu

Figure 18. Create Data Set options dialog

  o *Film loop.* This command allows users to animate the progress of the displayed particles through time and saves the output to an avi file.

o *Compute grid datasets.* This command allows users to convert the particle data in a region to a set of cells in a Cartesian grid. For example, the user may want to visualize the concentration of suspended particles over a Eulerian domain. By defining a grid in the grid module, the user can select this command, and SMS computes the concentration based on the number of particles in each cell of the grid, and the cumulative particle masses as a ratio with the depth and size of the cell. Additional data sets that are computed include the number of particles from each source in each cell and the average deposition thickness in the cell.

SUMMARY: Various features, tools, and analysis capabilities outlined in this document are designed to enhance the ability of engineers to run the PTM in the SMS. This technical note is applicable to Version 1.0 of PTM, and provides an overview of the main features of the interface necessary for accurate and efficient usage of the model. The PTM and SMS-based interface will evolve as the model is developed and applied in engineering applications. Therefore, the interface of the PTM will undergo revision. Feedback and suggestions from users on design, implementation, and usage of the present version of the PTM interface are welcome.

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> Demirbilek, Z., Smith, J., Zundel, A., Jones, R., MacDonald, N., and Davies, M. (2005). "Particle Tracking Model (PTM) in the SMS: I. Graphical Interface," *Dredging Operations and Environmental Research Technical Notes Collection* (ERDC TN-DOER-D4), U.S. Army Engineer Research and Development Center, Vicksburg, MS. An electronic copy of this TN is available from http://el.erdc.usace.army.mil/dots/doer.

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