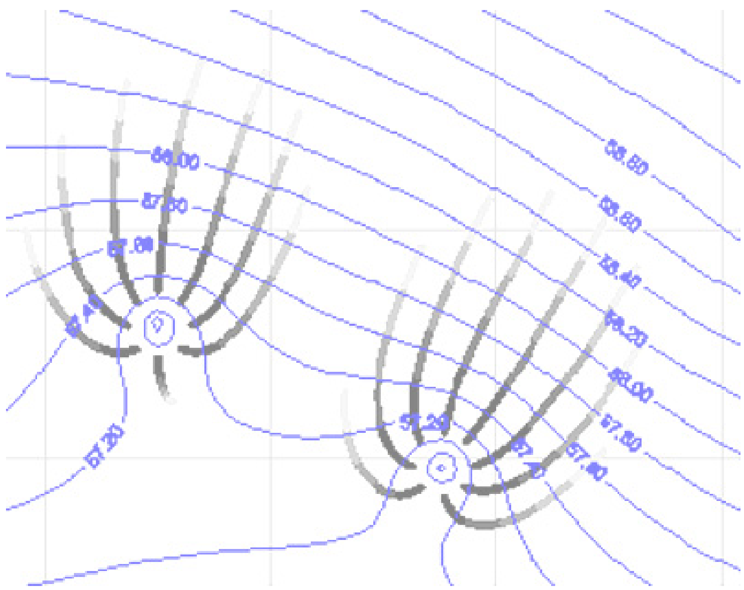
Version 3.0 - Beta

KT3D_H2O

A Program for Kriging Water Level Data using Hydrologic Drift Terms



User manual

Version 3.0 - Beta

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DESCRIPTION OF THE KT3D_H2O PROGRAM SUITE

Attachment 1:

KT3D_H2O v3.0 A Program for Kriging Water Level Data using Hydrologic Drift Terms: Theoretical Documentation

Attachment 2:

Documentation and Verification Package for TransientTracker

Introduction

KT3D_H2O Version 3.0 is a graphical user interface (GUI) that combines various programs to generate gridded maps of water level elevations, particle tracks and capture zones. These tools combine geosatistical and hydrological sciences to allow the user to generate map-based hydrogeologic analyses outputs without having to revert to numerical or analytical models.

KT3D_H2O is developed as a plug-in application under the open-source GIS foundation MapWindow. It allows the user to generate gridded maps of water level elevations that include the following elements that have important influence on the shape of the mapped surface and are usually ignored by other gridding software applications:

- Point Sink or Source of Known Strength: accounts for mounding (or drawdown) in response to injection (or extraction) at a known rate at one or more wells.
- Horizontal Line Sink or Source of Known Strength: account for mounding (or drawdown) in response to horizontal linear features of known extraction (injection) rate, such as interception trenches or infiltration galleries; and
- Circular Leaking Pond of Known Strength: accounts for the potentiometric response of a water table (unconfined) aquifer to infiltration through the base of a circular pond.

The available drift terms can be applied simultaneously, i.e. a single gridded surface may contain point sinks or sources, horizontal line sink or circular leaking pond. In addition, in order to account for heterogeneity, different groupings of the drift elements are possible so that scaling provided by universal kriging is performed independently on each group to obtain a best fit (e.g. wells located in a high transmissivity zone can be assigned to Point Sink Drift Term 1 and wells located in a low transmissivity zone are placed in Point Sink Drift Term 2).

These gridded surfaces can be used to complete the following types of hydrogeologic analyses maps for single or multiple events:

- maps of water level elevations;
- maps showing particle traces (particle tracking); and
- maps of particle capture (capture zone analysis including capture frequency maps)

About this Document

This document describes the various functions of the KT3D_H2O graphical user interface. Attachments 1 and 2 provide the theoretical documentation for the underlying codes: KT3D_H2O and Transient Tracker. This document constitutes a Beta version release that is not complete or fully tested.

Underlying codes

KT3D_H2O Version 3.0 is written in VB.Net and combines the latest version of linear-log kriging program KT3Ddll.dll and Transient Tracker. First version for kriging with linear-log drift, called KT3D_L1, is developed by modifying popular GSLIB KT3D kriging code then fortran program is compiled as a Dynamic Link Library (DLL), which is executed using a Visual Basic UI called "kt3d_loglin".

The MapWindow application is a free and extensible geographic information system (GIS) that can be used to distribute data to others, and to develop and distribute custom spatial data analyses. MapWindow includes standard GIS data visualization features as well as DBF attribute table editing, shapefile editing, and grid importing and conversion. MapWinGIS ActiveX includes a GIS API for shapefile and grid data with many built in GIS functions.

Supported Inputs and Outputs

The KT3D_H2O GUI supports importing data from Microsoft Excel versions 2000-2007 (*.xls, *.xlsx, *. xlsb and *.xlsm) files, Microsoft Access versions 2000-2007 (*.mdb and *.accdb) files, ESRI Shape Files (*.shp) and ASCII. It offers several post-processing options for the calculated grids:

Selected Output Format	**Grid Format**	**Particle Line Format** (1,2)
Surfer™	ASCII Surfer™ v7 Grid	
ESRI / ArcMAP™	ASC	ESRI Shape (SHP) file

1. Times associated with pathlines are written in units that correspond with the specified hydraulic conductivity units in the GUI's {Part.Track} tab.
2. All methods result in the production of the file "CAPTURE.OUT"
3. Appendix C describes the ASC grid format

Disclaimer

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The current release constitutes a Beta version that has not been fully tested.

Technical Support

Technical support regarding use of the graphical user interface can be obtained by writing to karanovicm@sspa.com.

Installing and starting KT3D_H2O

Installation Requirements:

- It is assumed that KT3D_H2O users already have some basic understanding of kriging techniques and GIS concepts.

- It is assumed that user already has installed the latest version of MapWindow, which can be downloaded at:
(http://www.mapwindow.org/download.php?show_details=1)

- The latest version of the MapWindow book can be purchased or downloaded free from http://www.lulu.com/ Also, the 1st edition of book is included in KT3D installation file

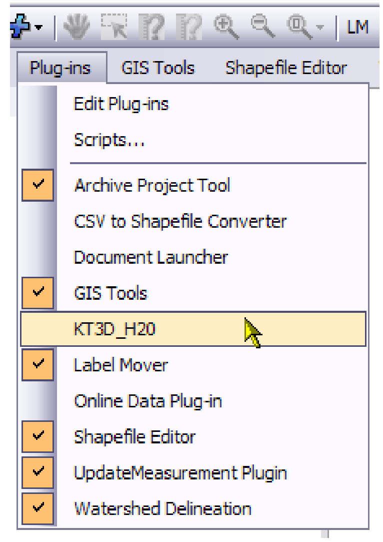
To install KT3D_H2O using the setup file, follow these three steps:

1. Download the installation program: KT3D_H20_Setup.exe from: www.sspa.com

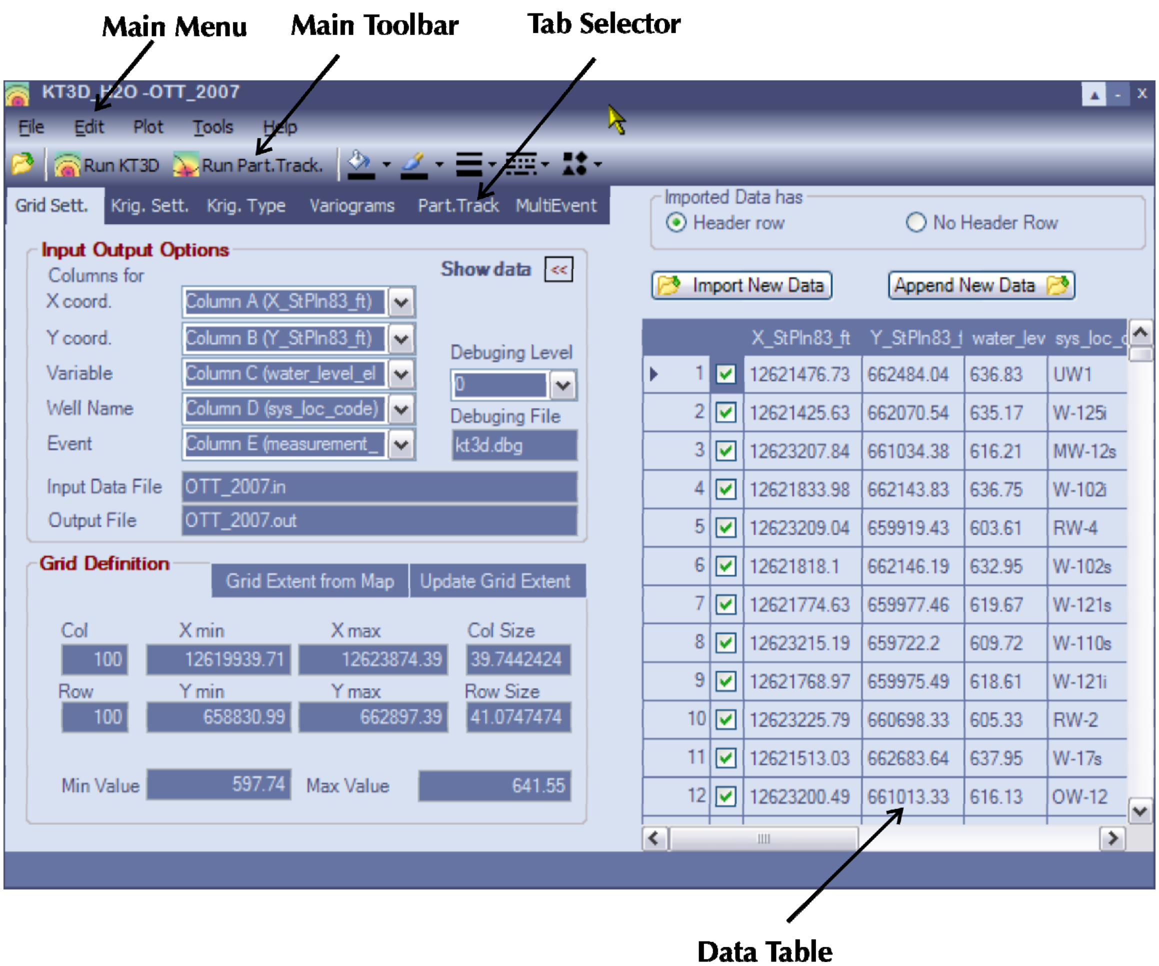
2. Run the installation program, following instructions on the screen. The destination folder must be the MapWindow root folder, usually "C:\ProgramFiles\MapWindow".

3. The setup program installs all necessary Dynamic Link Library files (dll's), user's manuals and sample files into appropriate MapWindow folders.

After installing KT3D_H20, open MapWindow. Click on "Plug-Ins" from the MapWindow toolbar, and select "KT3D_H20". This will add KT3D_H2O to the MapWindow toolbar. If "KT3D_H2O" is not listed under "Plug-Ins", make sure that the file "SSPA Tools.dll" exists in MapWindow plugins folder usually, "C:\ProgramFiles\MapWindow\Plugins\" or "C:\ProgramFiles\MapWindow\Plugins\KT3D_H2O".



The KT3D_H2O button should now appear on your MapWindow Menu bar. Click on this button to open the KT3D_H20 User Interface (UI):

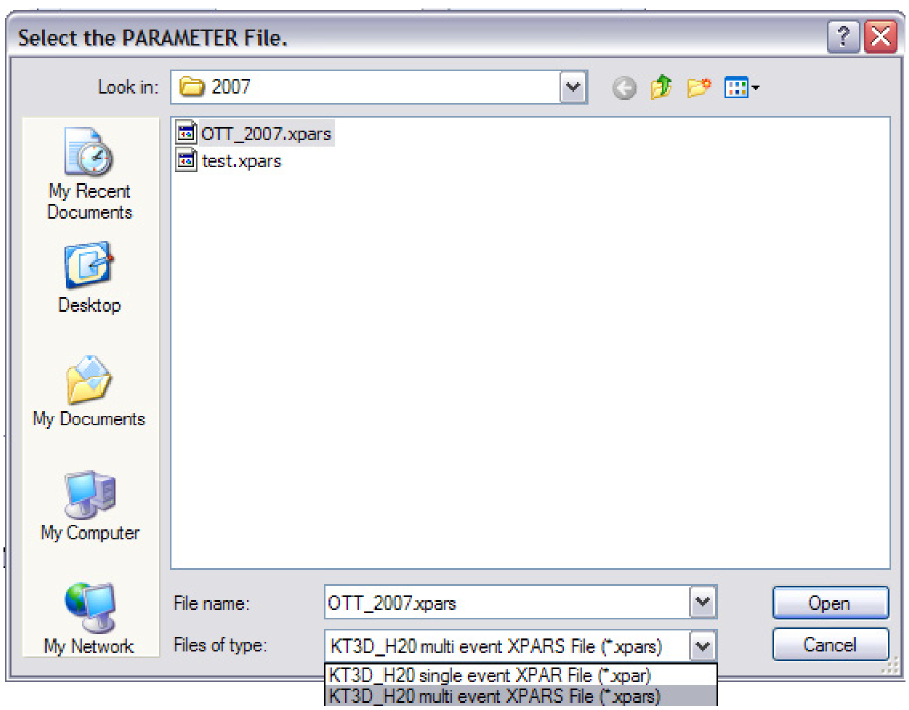


Creating a new project

In order to use KT3D_H2O, you first need to create a new project or open an existing one. There are two types of projects that can be used for the kriging: the **Single Event** type for the kriging one data set, and **Multi Event** type for kriging multiple data sets. The Single event type is used to create a single result; for example, a single map of overall average water elevation. The Multi Event type is used to create multiple results corresponding to multiple events; for example, this type would be used to create several maps, each showing water levels from a different sampling event.

To create a new project: At the KT3D_H20 main menu, select [File]-[New]. A dialog will open prompting you for a folder name, file name and project type. Select the folder where all data will be stored, then enter the project file name. For project type, select "KT3D_H20 single event XPAR File (*.xpar)" for a single event project or

"KT3D_H20 multi event XPARS File (*.xpars)" for a multi event project. Then click [Save].



To open an existing project: In the KT3D_H20 main menu, select [File]-[Open]. Navigate to the appropriate folder and choose the correct file type (*.xpar or *.xpars). Your project name should appear in the window. Select it and click [Open].

Kriging to Generate a Grid

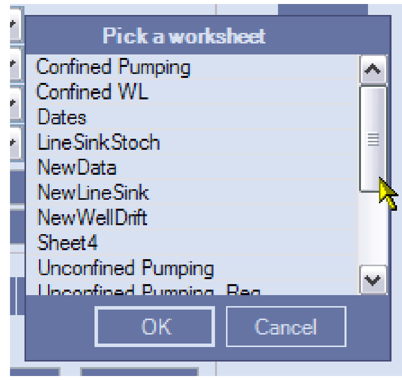
Preparing data

The following table lists the input parameters for KT3D_H2O and generate a groundwater elevation grid map. Appendix A describes the file formats:

Minimum Requirements			
Input type	***Supported input file type formats***	***Required components***	
		xpar file, single event kriging	***xpars, multi-event kriging***
XYZ data to krig (eg, water elevation measurements at wells)	Microsoft Excel (.xls,.xlsx,.xlsb, or .xlsm);Microsoft Access (.mdb or .accdb); ESRI shapefile (.shp); ASCII (.txt or .dat)	X, Y coordinate of each location Z-value at each location (variable to krig, e.g., water elevations) Location Name (e.g., well ID)	X, Y coordinate of each location Z-value at each location (variable to krig, e.g., water elevations) Location Name (e.g., well ID) Event date
Optional Drift Terms for Water Level Kriging			
Drift Type	***Supported input file type formats***	***Required components***	
		xpar or xpars projects	
Pond drift	Microsoft Excel (.xls,.xlsx,.xlsb, or .xlsm);Microsoft Access (.mdb or .accdb); ESRI shapefile (.shp); ASCII (.txt or .dat)	X, Y coordinate at the center of each pond Radius of each pond Sink strength for each pond Drift term flag for each pond	
Line Drift	Microsoft Excel (.xls,.xlsx,.xlsb, or .xlsm);Microsoft Access (.mdb or .accdb); ESRI shapefile (.shp); ASCII (.txt or .dat)	X, Y coordinates which define each line (minuimum two points) Sink strength	
		Drift term flag for each line	
		xpar file, single event kriging	***xpars, multi-event kriging***
Well Drift	Microsoft Excel (.xls,.xlsx,.xlsb, or .xlsm);Microsoft Access (.mdb or .accdb); ESRI shapefile (.shp); ASCII (.txt or .dat)	X, Y coordinate of each injection or extraction location Injection or extration rate at each location Injection or extraction location name (e.g., Well ID) Drift term flag for each location Indicator (boolean) if well is used for recovery*	X, Y coordinate of each injection or extraction location Injection or extration rate at each location Injection or extraction location name (e.g., Well ID) Drift term flag for each location Indicator (boolean) if well is used for recovery* Event Date

* Optional. Used for particle tracking only

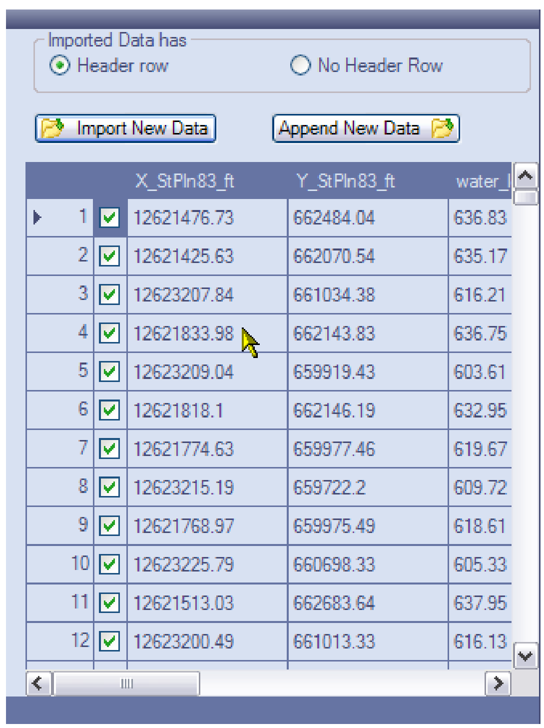
Importing data



To import new data, select {Grid Sett.} tab, and click on the button labeled “Show Data”, then click the 

button or [File]-[Import]-New Data Set]. Select the input data file type. KT3D_H2O supports importing data from Microsoft Excel (*.xls, *.xlsx, *. Xlsb and *.xlsm) files, Microsoft Access (*.mdb and *.accdb) files, ESRI ShapeFiles (*.shp) and ASCII (.txt or .dat) files with values separated by space, comma or tab. If an Excel or Access file is chosen then the worksheet/table/query selector dialog will appear.

Select the appropriate worksheet/table/query then click [OK]. Your data should appear in the data table.



By default the “Data Has Header Row” button is selected, if your data has no header row, click the “No Header Row” radio button.

Setting grid parameters

To set grid parameters, click on the {Grid Sett.} tab in the main menu. Parameters are set in the "Input Output Options" section. Input options for both single-event (.xpar) and multi-event (.xpars) projects include: XCoord, YCoord, Variable, and Well Name. By default, KT3D_H2O assigns the first column in your input data as X coordinate, second as Y coordinate, third as kriging variable and fourth as well name. Any input option column reference can be changed using the corresponding drop down menus. For single-event projects, there is an additional option for External Drift Variable. This column is not assigned by default and must be selected by the user. Kriging with External drift is not supported in Multi Event projects. For Multi Event projects, instead of External Drift Variable, there is an option for Event date. This column is not assigned by default and must be specified by the user. The data in this column must be in the form of a Julian date (e.g. "1/1/2008" or "January 1, 2008").

Grid extent can be updated in three ways:

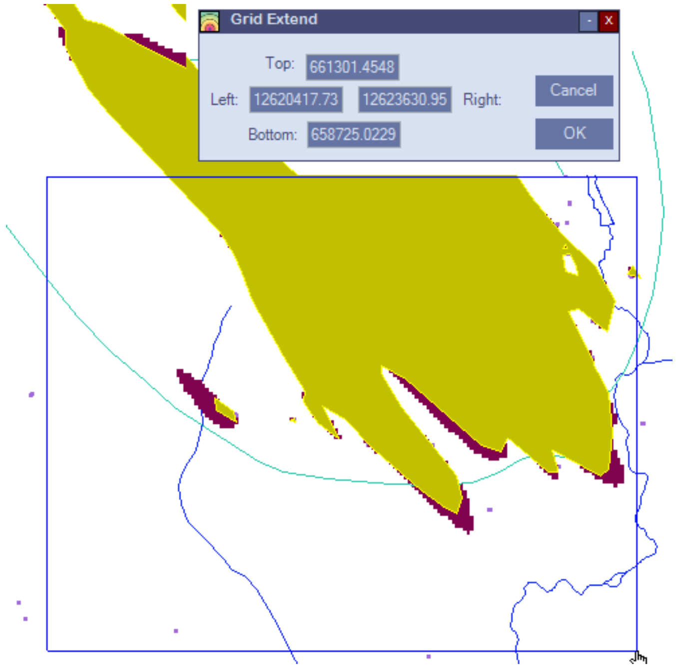
1. Entering values for Xmin, Xmax,Ymin and Ymax manually

2. By clicking the 

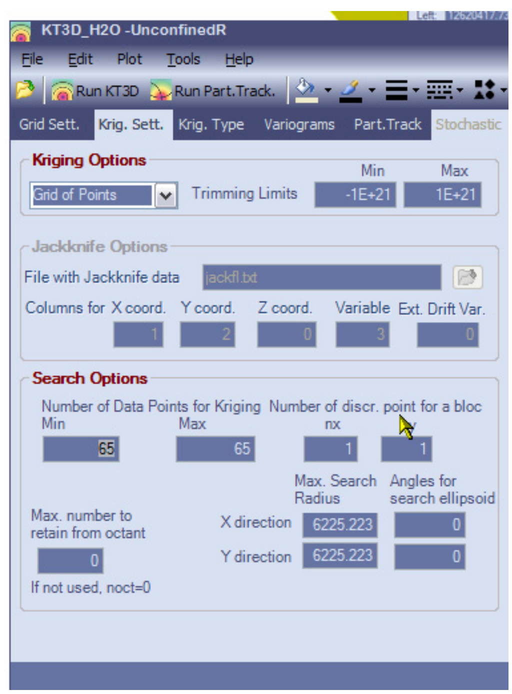
button. The program will analyze all values for X and Y coordinates of your input data and assigns minimum and maximum values for grid extent.

3. By clicking the 

button. You can generate the grid extent by drawing rectangle on the project map. Left mouse click to the start drawing and right mouse click to end drawing. Grid extent coordinates can be edited on "Grid Extent" dialog, Once you are satisfied with grid extent click [OK]



Setting Kriging parameters



To set kriging parameters, select the {Krig Sett.} tab. Three kriging options are available in the pull-down menu: regular kriging grid of points, Cross validation, and Jackknife. In cross-validation, actual data are dropped one at a time and re-estimated from some of the remaining neighboring data. Each datum is replaced in the data set once it has been re-estimated. The term jackknife applies to resampling without replacement, i.e. when alternative sets of data values are re-estimated from other nonoverlapping data sets.

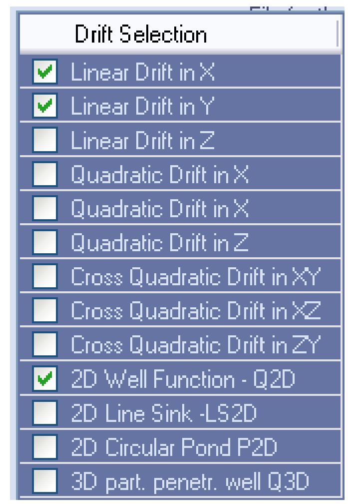
For detailed information of kriging parameters on this tab please refer to the GSLIB User's Guide book or visit the website at http://www.gslib.com/gslib_help/kt3d.html

Selecting kriging types and drifts

To set kriging type, trend indicator or drift options, click on the {Krig.Type} tab.

Kriging Type and Trend Indicator: Kriging type and trend indicator can be selected from the pull-down menus in the {Krig.Type} tab. For more information on the theory and implementation of different kriging types and trend indicator options, refer to the GSLIB User's Guide.

Drift Selection: The standard KT3D program includes nine drifts options. In KT3D_H2O, three additional drifts are added and fully supported: the 2D Well function (Q2D), the 2D Line Sink (LS2D) and 2D Circular Pond (P2D). These drift terms are described below. A thirteenth drift, 3D partial penetrating well drift (Q3D), is under development and is not yet supported. See Attachment 1 for a complete theoretical description of the additional drift terms included in KT3D_H2O.

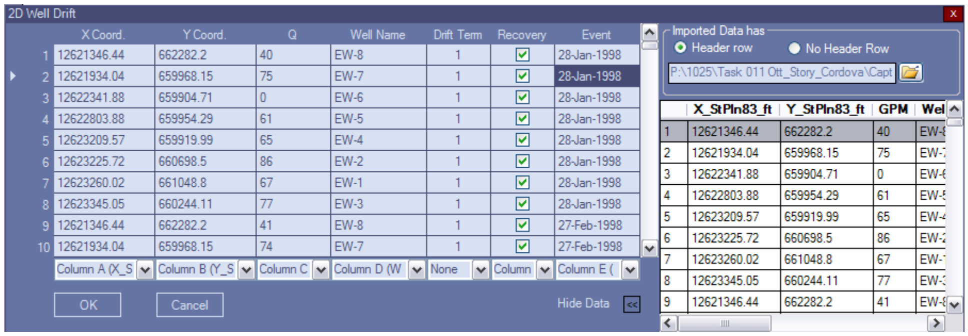


2D Well function drift

The approach of kriging ground water levels measured in the vicinity of pumping wells using a regional-linear and point-logarithmic drift, the latter derived from the Cooper-Jacob and (or) the Thiem equation, is fully described by Tonkin and Larson (2002). (See Appendix 1). Following its publication, the "linear-log" drift was added to the GSLIB KT3D program, here called "2D Well Function (Q2D)". This drift is strictly compatible only with 2-D kriging and can be used with any of the standard drifts included with KT3D.

To include the 2D well function drift, click on the check box labeled "2D Well function (Q2D) If well drift data have not been imported previously, a file selector dialog will open. Supported input file formats Microsoft Excel (*.xls, *.xlsx, *. Xlsb and *.xlsm) files, Microsoft Access (*.mdb and *.accdb) files, ESRI ShapeFiles (*.shp) and ASCII (.txt or .dat)

Navigate to the appropriate input file and click [OK]. This will import the well drift data into KT3D_H20 and open the 2D Well Drift dialog. To view your original data or to select a different input file, click "Show data" at the bottom right of the dialog window.



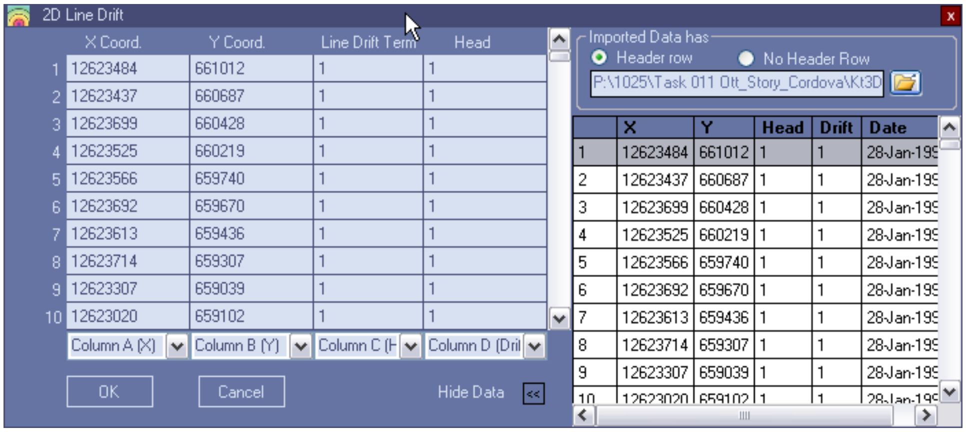
By default X and Y coordinates are the first and second columns in your input data set, pumping rate is the fourth column, well name is the fifth, and drift term in sixth. This can be changed by selecting the appropriate columns using drop down menus under each of data table columns. Selecting the value "None" in the drift term drop down menu will generate number one (1) for all wells as a drift term. If you are running a multi event project, an additional field called "Event" is available. The events should be a Julian date, and should correspond to the events in your water level input data.

Recovery column values (True/False) are used in particle tracking procedure, to define if well is used to determine capture zones analysis (default value is True).

Once imported, the well drift data may be edited in the Well Drift dialog. To exclude the well drift, select the whole row by clicking on the row number and press "Delete" key on your keyboard. Confirm completion of well drift data editing by clicking [OK]. Well drift data can be edited or changed at any time by selecting [Edit] from the KT3D_H20 main toolbar and then selecting [2D Well Drift] from the pull-down menu.

2D Horizontal line sink/source drift

To add the effect of horizontal linear features click on 2D Line Sink check box or select [Edit]>[2D Line Drift]. The 2D Line Drift dialog will appear.

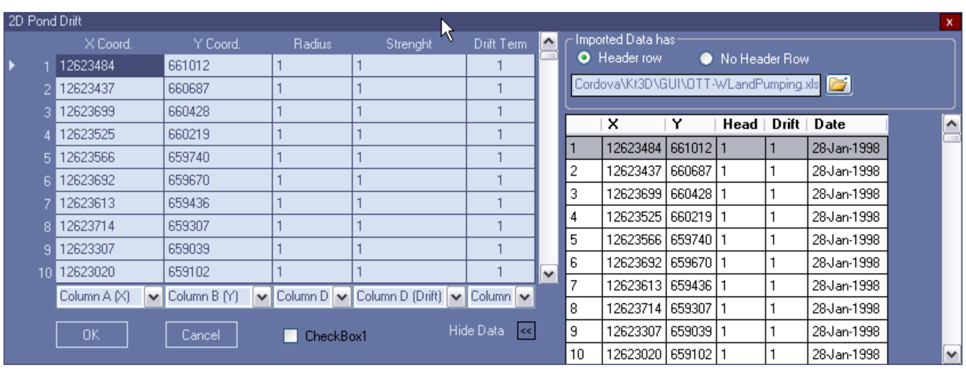


Click the [Show Data] button to open the data import dialog. Choose the appropriate input file and click [OK]. The table to the left of the dialog will fill in with the input data. Select the appropriate columns for coordinates, drift term, and head. Note that Drift Term and Head must be numeric values, and there is no event date column. Single imported data set will be used for all kriged events.

Click [OK] to confirm completion.

2D Circular pond

Two dimensional circular pond drift can be added by clicking on 2D Circular Pond check box or select [Edit]>[2D Pond Drift]. The 2D Pond Drift dialog will appear.

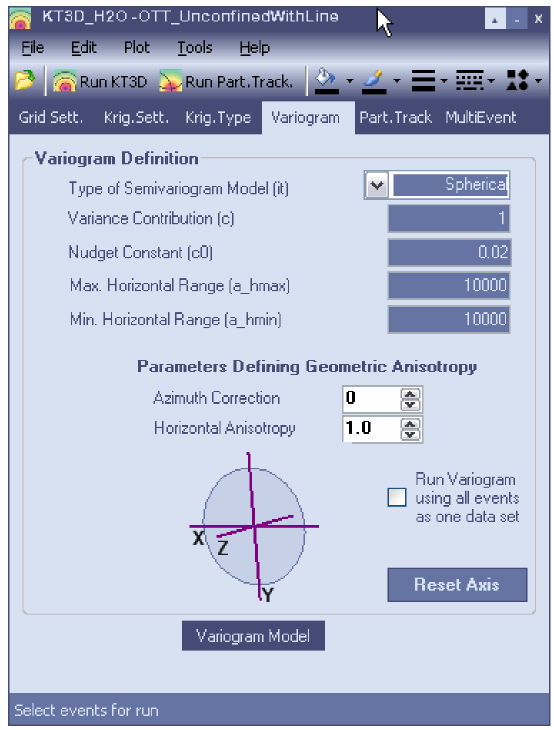


Click the [Show Data] button to open the data import dialog. Choose the appropriate input file and click [OK]. The table to the left of the dialog will fill in with the input data. Select the appropriate columns for coordinates, radius, strength and drift term. [OK] to confirm completion.

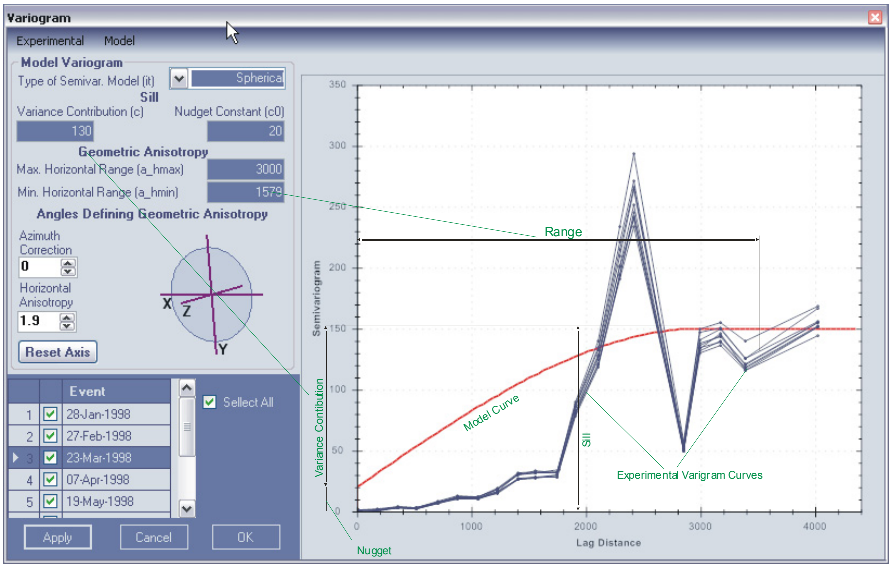
Setting variogram parameters

At the {Variograms} tab, the user can set and view variogram parameters. In this version of KT3D_H2O only one variogram at a time may be selected. (This differs from original GSLIB KT3D which accepts "unlimited" number of variograms. For the detailed explanation of variogram parameters please refer to the GSLIB Book.

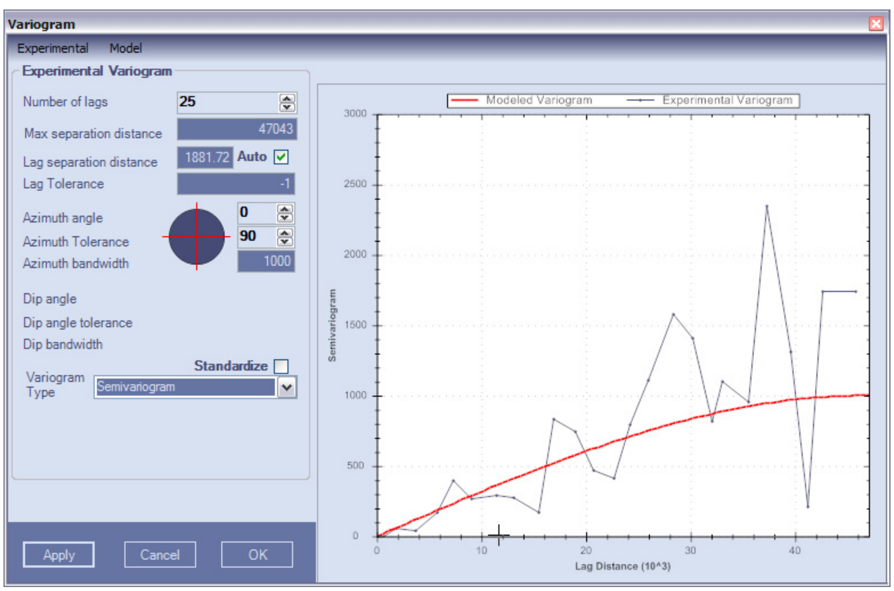
For variogram modeling, KT3D_H2O uses the GSLIB programs "gamv" and "vmodel". To model single the variogram, click on the [Variogram Model] button which opens variogram dialog on variogram modeling page. In case of multi event projects there are two options to model variogram: The first option is to run Variogram model using all data as a one data set and the second options is run Variogram model using each event as a separate data set. The Event Selector dialog will appear. Select the appropriate events and click [OK].



The UI automatically calculates the experimental variogram(s) model (using "gamv") and plots them on variogram plot as a blue line(s)).



After adjusting model parameters it is necessary to click on [Apply] button to recalculate model (using GSLIB "vmodel" program) and refresh the plot. At any time you can switch to the experimental page and adjust experimental parameters. After parameters are adjusted click on [Apply] to execute "gamv" program and refresh the variogram plot.



After the appropriate parameters are entered and "best fit" is achieved, click the [OK] button to return to variogram page.

Running the Kriging

Before kriging, it is recommended that you save your MapWindow project file and your KT3D parameter file. To execute the KT3D kriging program click the 

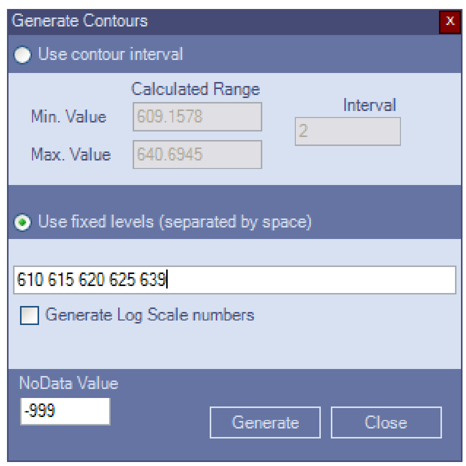
button. You can terminate kriging at any time by pressing the [ESC] key.

Single event kriging

To run kriging, click the 

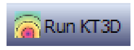
button. After kriging is finished, the UI will prompt you to enter an ASCII grid file name. The grid will be saved in the same directory as the .xpar or .xpars file and imported to the MapWindow project map. MapWindow automatically generates a *.bmp file for viewing purposes and an *.mwleg file, which is XML file that contains layer legend information. KT3D_H2O also generates an XML file (*.xasc) which contains all parameters and all input data used for the kriging. Data from XML file can be imported at any time selecting the [File]-[Import]-[Xml Data].

To generate contours select [Plot] then [Contours]. A file selection dialog will appear. Select the appropriate grid file and click [OK]. The "Generate Contours" dialog will appear.

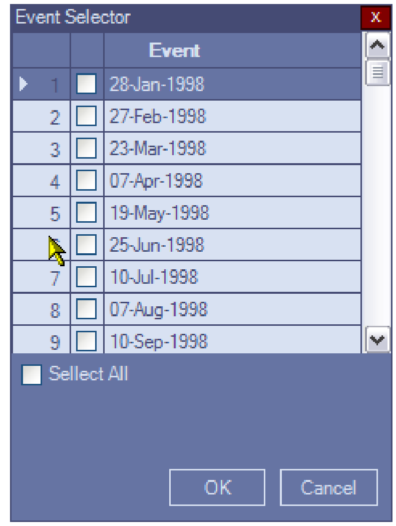


Contours levels may be set two ways. Fist, you may set the maximum and minimum values and contour interval. By default, the maximum and minimum contour values are determined from the grid, but these values may also be entered manually. Second, you may specify levels by entering level values separated by a single space in the text box. After you have determined the contour levels, click the [Generate] button. This will generate a shapefile (.shp) showing the contours. You will be prompted for the shapefile name, and the location where the file will be saved. By default, this is the project directory. Once you click [Save] the shapefile will be displayed in the MapWindow project.

Multi Event kriging

To run kriging, click the 

button. The Event Selector dialog will appear. Select the appropriate events and click [OK]. After each event is kriged you will be prompted to enter the ASCII grid file name. To avoid repeating this step, click on [Tools]-[Project Settings], then check “Overwrite Existing Files”. If this option is selected, the UI will generate and use default ASCII grid filenames and save them in the project directory. The default file name is constructed as: project file name + “_” + event date (for example, “newproject_28-Jan-1998.asc”). All kriged grids will be added to the project map. If you don’t want your kriging grid files to be added to the map, click [Tools]-[Project Settings] and uncheck “Add Results to Map”. It may be necessary to do this if you have a large number of kriging events because plotting each map can significantly slow down your system.



To generate contours in multi event projects, select [Plot]-[Contours]. The Event Selector dialog will appear. Next to the Event is the column “GridFile” populated with the default equivalent ASCII grid file name. If the ASCII file name or directory was anything other than the default assigned by the UI, then it is necessary to select the grid file manually. To do this, right click in the event “GridFile” cell. You will be prompted to select another ASCII grid file which will be used for contouring in that Event.

Select desired events and click [OK]. Contour shapefiles will be created for each event. See Single Event Contouring for a full description of the contouring process.

Kriging output results also can be viewed by plotting nodal values, Select [Plot] then [Kriged Nodal Values], select event and UI will generate point shape file with X and Y coordinate, row, column and kriged value at every node of your grid.

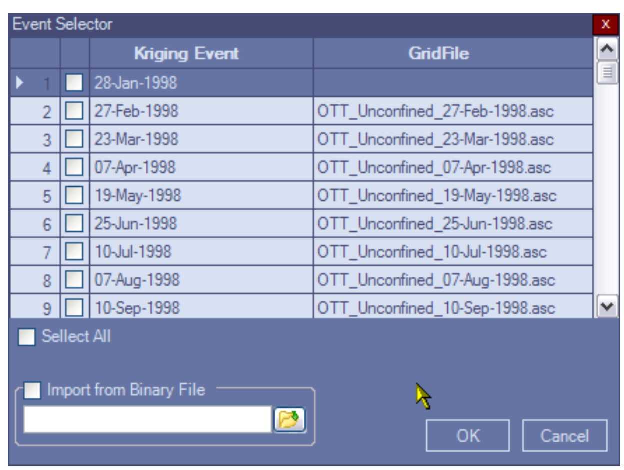
Exporting kriging results

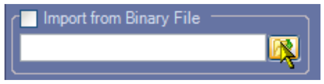
Kriging results can be exported as a binary file (*.kbf). To do that select [File]-[Export]-[KT3D_H2O Binary file] (for file format see Appendix B). Then in "file type" dropdown menu select "KT3D_H2O Kriging Binary File (*.kbf)". Enter the file name. For Multi Event projects, the Event Selector Dialog will appear. Select event grid files you wish to export.

To export kriging results as a Surfer ASCII grid file select [File]-[Export]-[ASCII Surfer Grid]. For a Multi Event project, the Event selector dialog box will appear. Select the Event grid files you wish to export. For each event you will be prompted to enter the Surfer ASCII grid file name and location. To skip this step, click on [Tools- Project Settings] then check "Overwrite Existing Files". If this option is selected, the UI will generate and use default Surfer grid filenames and save them in the project directory. The default file name is constructed as: project file name + "_" + event date (for example, "newproject_28-Jan-1998.grd"). Surfer grid files can also be automatically generated during Multi Event kriging. To do this, go to the {Multi Event} tab, check "Generate Surfer grid file during multi-event run". Note this option must be selected before kriging is performed.

Importing kriging results

Kriging results can be imported at any time by selecting [Plot]-[Color Flood]. For Mulit-Event projects, a "Event Selector" dialog will appear. If all files have default file names, the "Gridfile" cell next to each event will be populated with the corresponding ASCII grid file name (*.asc). Alternately, you can select any ASCII grid file to plot by right-clicking in the "Gridfile" cell next to the Event. A file selector dialog will appear. Choose the appropriate grid file (*.asc) and click [Open].

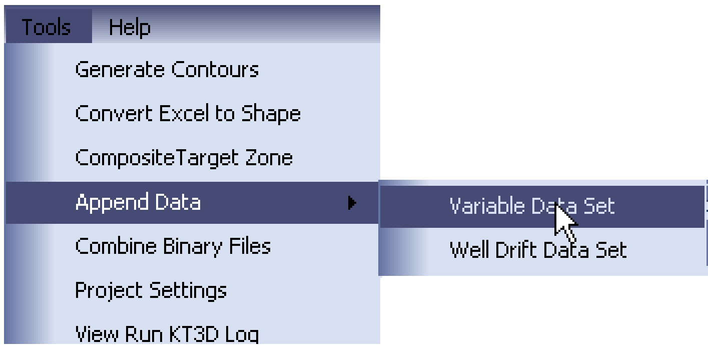


To import kriging results from a kriging binary file, click on “Import from Binary File” checkbox 

then from File open dialog select “Kriging binary file”. The UI will read all saved events in the binary file, the Event selector dialog will appear. Select which events to plot. This will generate new ACII grid files for each selected event. You will be prompted to enter a file name for each. To skip this step, before importing the binary file, click on [Tools]-[Project Settings] in the main KT3D_H20 window. then check “Overwrite Existing Files”. If this option has been selected when the binary file is imported, the UI will generate and use default ASCII grid filenames for each event and save them in the project directory. The default file name is constructed as: project file name + “_” + event date (for example, “newproject_28-Jan-1998.asc”).

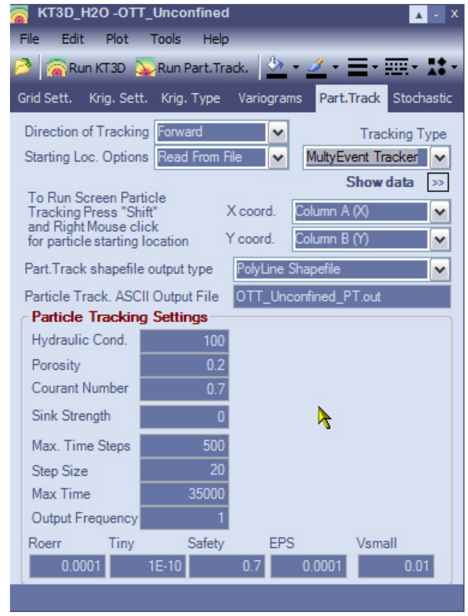
Append new Events

To append a new sampling event(s) to an existing Project data set, click [Tools]>[Append Data] then select the appropriate dataset to append. In the dialog form select appropriate columns as explained in the “Importing Data” section. To confirm that your new data set is imported correctly, click [OK]. The new data will be appended to the end of the data table.



Particle tracking

The grids generated as described in the previous section can now be used to generate a particle tracks. Particle tracking is performed in KT3D_H2O using TransientTracker (Attachment 2). It supports the approximate evaluations of historic and future contaminant migration; of hydraulic capture zones developed by pump-and-treat type remedies; and other analyses that benefit from the ability to track particles on a surface. The particle tracking utility has been adapted to use the program TransientTracker as a processing engine while KT3D_H2O is used to generate ASCII input files and for post-processing TransientTracker outputs.



All particle tracking settings are in the {Part.Track} tab. Here you can set particle starting locations, tracking type, tracking parameters and output type.

Setting particle tracking parameters

The following parameters are required to perform particle tracking:

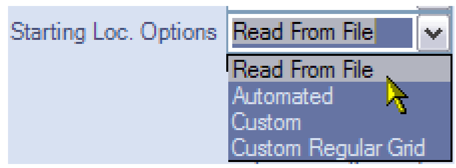
Input type	***format***
Hydraulic Conductivity in Aquifer	Entered as single numeric value in GUI
Porosity in Aquifer	Entered as single numeric value in GUI
Starting locations of particles	May be specified in using GUI as described; or imported from an external file. Supported file types: Microsoft Excel ,or ASCII text including XY coordinates of each starting location; or an ESRI shapefile (.shp) showing all starting locations.
Results of KT3D water level kriging	.asc files generated by KT3D. When KT3D is run, these files are saved automatically in the same directory as the .xpar or .xpars file, and are imported automatically before particle tracking is run.

For practical reasons all input parameters which contain a time component must use the unit “days”.

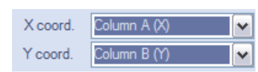
For explanation particle tracking parameters please refer to the included Transient Tracker documentation (Attachment 2).

Setting particle starting locations

There are five options to generate particle starting locations:

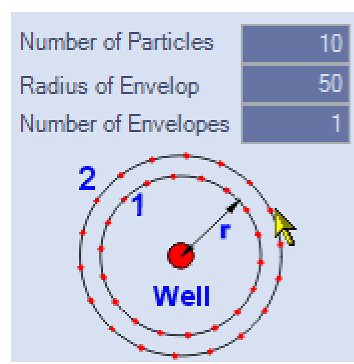


a. **Read from File**: To import starting locations from a file, under the {Part. Tab}, click 

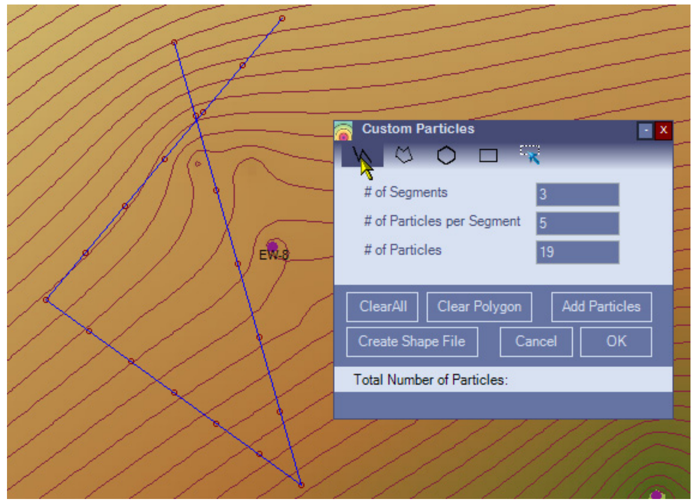
button to expand the KT3D_H2O main window. Then click Open file button next to "Start. Loc File". 

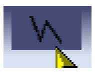
Select the type of input file (ASCII, Excel or Shapefile). After data are imported, use column selector dropdowns to select column for X and Y coordinate.

b. **Automated:** For projects using a 2D well drift, there is an option to generate particles around each well in circular envelopes. Enter the number of particles per envelope, number of envelopes, and radius of envelopes. For example, if the radius of the first envelope is 50 ft, then the radius of the second is 100; the radius of the third envelope is 150 ft, and so on. This option can be executed only using backward tracking.

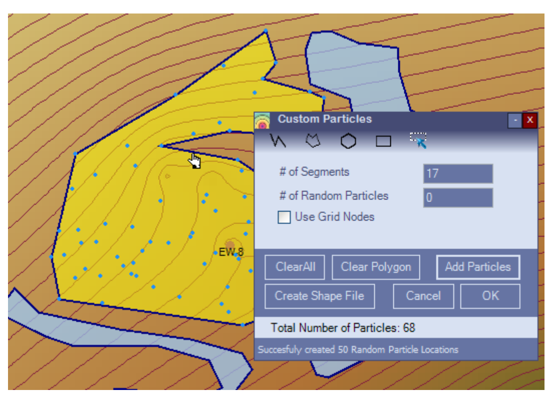


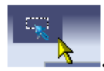
c. **Custom:** This option allows you to generate particle starting locations by drawing polylines or polygons, or by selecting shapes from existing polygon shape files. To open the Custom Particles dialog, select "Custom" from the pull-down menu next to "Starting Loc".



1. To draw a polyline: Select the {polyline}  tab on dialog menu. In the Project Map, left click to begin the line, and right click to end it. In the Custom Particles dialog, type in the desired number of particles per segment. The total number of particles will be calculated based on the number of segments in the polyline and the number of particles per segment. After you have drawn the polyline and set the number of particles per segment, click [Add Particles]. Red dots will be converted to blue, indicating that those locations are saved in memory. To add more particles simply draw another polyline.

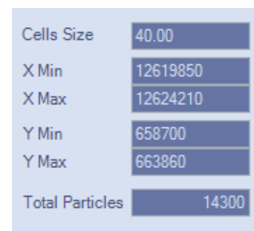
2. To draw a polygon: From the Custom Particles toolbar select the shape of polygon (irregular, n- sided regular or rectangular). Left click to start the polygon and right click to end it. To draw a square, select the rectangle tool and hold down the Ctrl key while drawing the rectangle. Particles may be generated inside the polygon one of two ways: either enter the number of particles next to "# of Particles", which will generate the set number of particles at random locations inside the polygon; or check "Use Grid Nodes" to generate particles at all kriging grid nodes inside the polygon.



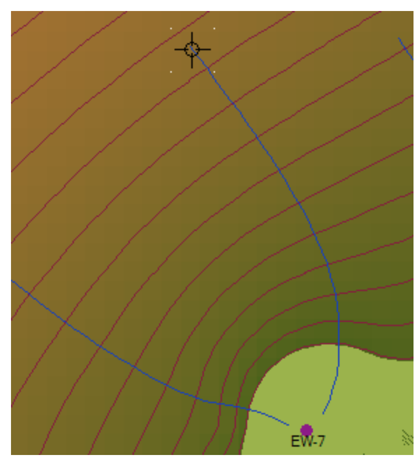
To use existing polygon shape file: In the Custom Particles dialog, select the shapefile import tab from the dialog toolbar . Select the polygon shape file from the legend then select desired shape. Enter number of particles as explained in section 2 above and click [Add Particles].

To generate a point shapefile from generated particle locations, click [Create Shape File]. After generating particles click [OK]. The UI will populate a particle worksheet with particle coordinates.

d. **Custom Regular Grid:** Select "Custom Regular Grid" from the pull-down menu next to "Starting Loc. Options". Enter X and Y coordinates and cell size. Default values are grid extents used in the kriging.



e. **Quick "screen" particle tracking:** For single event projects, hold down the Shift key (cursor will change to the target shape) and click with right mouse button at the particle starting location on the map. The program will instantly run particle tracking using existing particle tracking parameters. For Multi-Event projects, this option is only available using transient tracking. In the {Part. Track} tab, select "Transient Tracker". As with single-even projects, hold down the shift key and right click on the starting location on the map. The event selector dialog will appear. Select the grids to be used in transient tracking. The particle will be tracked along the selected grids according to the specified step size until the last date in the Event Selector Dialog ("End Time for Transient Tracker"). By default, this is the current date. More information on transient tracking is available in the attached Transient Tracker documentation (Attachment 2).



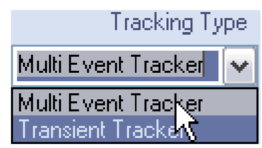
Running particle tracking

1. To run particle tracking for a single event project: set up particle starting locations as described in the previous section. Select particle tracking shapefile output type (point or polyline) and define particle tracking parameters. Then from the Mapwindow legend, select kriged grid file. In the main KT3D_H20 toolbar, click the "Run Part. Track" button. 

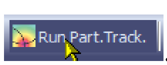
. After tracking is finished, you will be prompted to enter the path and output shapefile name. The output shapefile will be saved in the specified directory and added to the project map. Note: the grid you selected before running particle tracking the first time will remain active until you select a new grid. There is no need to select the grid each time you run particle tracking.

2. Multi event project

Two types of tracking are available for Multi Event projects: **Multi event** and **Transient** tracking.



Multi Event: In the {Part. Track} tab, under "Tracking Type" select "Multi-Event". Define particle tracking parameters and click the "Run Part. Track" button. The Event Selector dialog will appear. Select the appropriate event grid files and click [OK]. KT3D_H2O will perform particle tracking on each grid file individually using the specified particle tracking parameters for each event and also output files will be generated for each event.

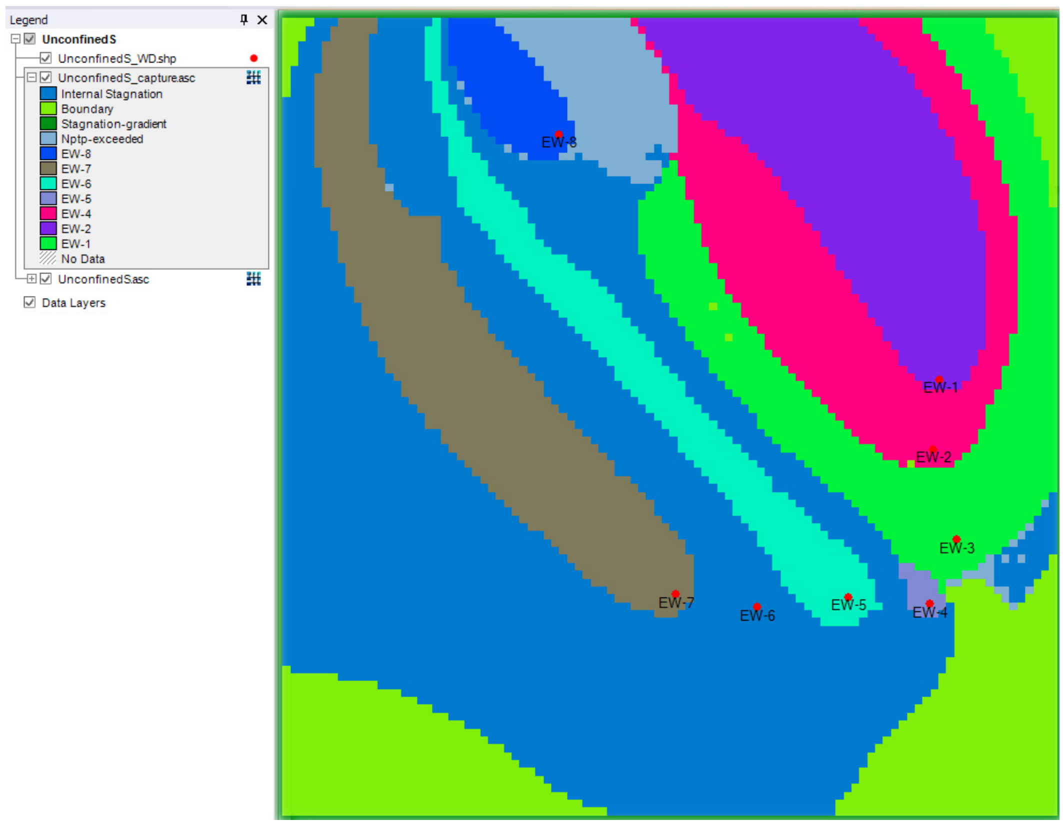
- **Transient Tracker:** In the {Part. Track} tab, under "Tracking Type" select "Transient Tracker". Define particle tracking parameters and click the "Run Part. Track" button 

. The Event Selector dialog will appear. The column "GridFile" is populated with the corresponding event

default ASCII grid file names, any grid files may be selected by right clicking on the event GridFile cell. Check the appropriate events kriged grid files. The bottom of the Event Selector dialog contains an event called “End Time for Transient Tracker”. Enter the date that transient tracking stops. By default, this is the current date. This date may be changed manually, or may be chosen from the calendar. To view the calendar click slowly two times on the “End Time for Transient Tracker” Event Date cell. Transient tracking will be performed along the selected grids from the first date selected to the specified end date. Step size must be specified in the particle tracking parameters, and must be in units of “days”. For more information on the transient tracking process, see the attached Transient Tracker documentation (Attachment 2).

Hydraulic Capture Zone analysis

Hydraulic Capture Zone analysis records the fate of particles during tracking simulation. TransientTracker (Attachment 2) includes functionality for removing particles at the margins of the grid domain; at stagnation zones; at sinks when forward tracking. The program records the fate of particles in an ASCII summary file. The contents of this file is used by KT3D_H2O to illustrate capture zones. This section describes how to use KT3D_H2O to generate capture zone maps and capture frequency maps.



• Hydraulic capture zones: In the {Part. Track} tab under "Starting Loc. Options, select "Custom regular grid" and under "Tracking Type" select Multi Event Tracker". Define particle tracking parameters and click "Run Part.Track" button 

. After particle tracking is finished, a capture ASCII grid file is generated. This file contains an array of integers which represents the different extraction wells, boundaries, and other types of zones, or sinks where a particle was removed from particle tracking. KT3D_H2O converts those integers into zone an explanation shown in the MapWindow legend. By default particle pathlines shapefiles are not generated during hydraulic capture analysis. This option can be selected by checking the "Generate Particle Tracking Shapefiles" box in the {Part. Track} tab 

.

- Capture Frequency map: For Multi Event projects, there is an additional option to calculate a capture frequency map. This map describes the number of times a particle was removed at an extraction well compared to the number of events calculated (i.e., the fraction of capture for each particle). For example, frequency of 0.5 indicates that during all the events for which capture zones were calculated, the particle was captured by an extraction well 50% of the time. This suggests that on the basis of the measured water levels, the assumed measurement errors, and the linear-log drift gridding approach employed, a particle originating from the given location would be captured by the combined pumping of extraction wells about 50 percent of the time. Hence, these maps illustrate the relative frequency with which particles of groundwater are captured under the varying conditions represented by different water level events.

A capture frequency map may be generated two ways. First, it will be generated automatically at the end of a capture zone analysis. After tracking has been completed for all events, a prompt will appear asking if you want to save the capture frequency map. Specify the path and file name and click "Save". Second, a capture frequency map may be created from the combination of any capture grid files. Select [Plot]-[Frequency Map] then select desired capture zone analysis gridfiles. Specify the path and file name and click "Save". The capture frequency map will be automatically added to the MapWindow project map.

Exporting Hydraulic Capture Zone analysis results

Capture Zone analysis results can be exported and saved as a binary file (*.cbf) (for file format see Appendix B). To do that select [File]-[Export]-[KT3D_H2O Binary file]. Then, in file type dropdown menu, select "KT3D_H2O Capture Binary File (*.cbf)". Enter the file name. For Multi Event projects, the in the Event Selector dialog box will appear. Select the event capture grid files you wish to export.

References

Deutsch, C., and Journel, A., (1992). GSLIB: Geostatistical Software Library and User's Guide. Oxford University Press, 340 pp.

Tonkin, Matthew J., and Larson, Steven P., 2002. "Kriging Water Levels with a Regional-linear and Point-logarithmic Drift". Ground Water, March/April 2002.

MAP WINDOW Desktop User Guide. http://www.mapwindow.org/wiki/index.php/MapWindow:Desktop

Appendix A

KT3D_H2O Input Formats

KT3D_H2O supports importing data from Microsoft Excel versions 2000-2007 (*.xls, *.xlsx, *. xlsb and *.xlsm) files, Microsoft Access versions 2000-2007 (*.mdb and *.accdb) files, ESRI Shape Files (*.shp) and ASCII (.txt or .dat) files with values separated by space, comma or tab.

Water Level data

KT3D_H2O required following set of variables in input data: First line is assumed to be header line for example: "X Y WL WellIDDate" then for each measurement line with XC(i), YC(i), Value(i), OID(i), Event(i)

	Variables
1	*Header Line*
2	XC(i), YC(i), Value(i), OID(i), Event(i)
	Where this line is repeated n measurements times.

The table below provides explanation of the variables used in KT3D_H2O input data.

XC(i)	X coordinate of the object (i)
YC(i)	Y coordinate of the object (i)
Value(i)	Kriging variable (i)
OID(i)	Name of the object (i)
Event(i)	Date of the event (Required for Multi Event projects)

By default, KT3D_H2O assigns the first column in your input data as X coordinate, second as Y coordinate, third as kriging variable and fourth as an object name. Any input option column reference can be changed using the drop down menus. For multi-event projects, a fifth variable, "Event" is required in format of Julian date (for example 01/01/2004).

Well drift data

Data defining locations and characteristics of each well used as a well drift should be provided in following format

	Variables
1	*Header Line*
2	*qxx(i), qyy(i), qqq(i), idtwell(i), qdrift(i), qtype(i), wellname(i), qevent(i)* where this line is repeated nwells times.

The parameters listed above have the following definitions.

NWELLS	KT3D_H2O will read file to the end, so no need to specify the number of wells. Lines begin with character "#" are considered as comment lines.
qxx(i)	X –coordinate of the well *i*
qyy(i)	Y –coordinate of the well *i*
qqq(i)	Pumping rate of the well *i* for the current event
wellname(i)	A name for the well
qdrift(i)	Drift term for well *i*
qtype(i) --	Specify the well as recovery (R) or not recovery (N) Used in capture zone analysis.
qevent(i)	Event Date in format of Julian date

Line Drift Data

LINEFILES(i): These files define the locations and characteristics of sink line segments. They are simple ASCII files and provide information in the following format.

Variables

1 *Header Line*

2 *lxs(i),lys(i),lind(i),lval(i)* where this line is repeated NLIN times.

The parameters listed above have the following definitions.

Lx(i) --	X location of point(s) i
Ly(i)--	Y location of point(s) i
Ldrift(i) --	Indicator of line sink/source drift term
Lval(i) --	Head value for the line feature.
Levent(i)--	Event date in format of Julian Date

Pond Drift Data

Pond Drift File: This file defines the locations and characteristics of circular and should be provided in the following format.

Variables

1 *Header Line*

2 *pX(i),pY(i),pRadius(i),pStrenght(i),pDrift* where this line is repeated by number of ponds.

The parameters listed above have the following definitions.

pX(i)	Pond center X coordinate
pY(i)	Pond center Y coordinate
pR(i)	Pond Radius
pStrenght(i)	Pond Strength
pDrift(i)	Indicator of pond drift term

For detailed information about each input parameter please refer to the Attachment 1.

Appendix B Binary File Formats

Kriging Binary file (*.kbf) and Capture Binary file (*.cbf) have identical structure, for the practical reasons they have different extensions. Binary file has one header section and "unlimited" grid array sections.

Data types used in binary files:

Type	**Description**
long	32 bit signed integer
double Text	64 bit double precision floating point value 1 bit

Header section describes dimension of 3D array and contains all the data for defining the grid

Element	**Type**	**Description**
nLay	long	number of layers in the grid (nlay=1)
nRow	long	number of rows in the grid
nCol	long	number of columns in the grid
xLL	double	X coordinate of the lower left corner of the grid
yLL	double	Y coordinate of the lower left corner of the grid
Rotation	double	not currently used
BlankValue	double	nodes are blanked if equal to this value
Txt	Text	Some file description 50 characters long.
xSize(ncol-1)	double	One dimensional array representing spacing between adjacent nodes in the X direction (between columns)
ySize(nRow-1)	double	One dimensional array representing spacing between adjacent nodes in the Y direction (between rows)

For each grid data in grid array section binary file contains:

Element	**Type**	**Description**
EventDate	Long	Event date in format of number of days counted from 1900
Grid(nLay,nRow,nCol)	Double	Grid Array

The grid values are stored in row-major order starting with the maximum coordinate. The first grid value in the grid file corresponds to the upper left corner of the map. The second grid value is the next adjacent grid node in the same row (the same Y coordinate but the next higher X coordinate).

Appendix C ArcInfo ASCII Grid Files Formats

ArcInfo ASCII Grid files [*.asc] contain seven header lines that provide information about the size and limits of the grid, followed by a list of Z values. The fields within ASCII grid files must be space delimited.

The listing of Z values follows the header information in the file. The Z values are stored in row-major order starting with the maximum Y coordinate. The first Z value in the grid file corresponds to the upper left corner of the map. The second Z value is the next adjacent grid node in the same row (the same Y coordinate but the next higher X coordinate). When the maximum X value is reached in the row, the list of Z values continues with the next higher row, until all the rows of Z values have been included.

The general format of an ASCII grid file is:

Element	**Description**
ncols ncol	number of columns in the grid
nrows nrow	number of rows in the grid
xllcenter X	X coordinate of the lower left center of the grid cell
yllcorner Y	Y coordinate of the lower left center of the grid cell
dx xsize	Grid cells size in X direction
dy ysize	Grid cells size in Y direction
Nodata_Value Nodata	nodes are blanked if equal to this value
Grid(nRow,nCol)	Grid Array

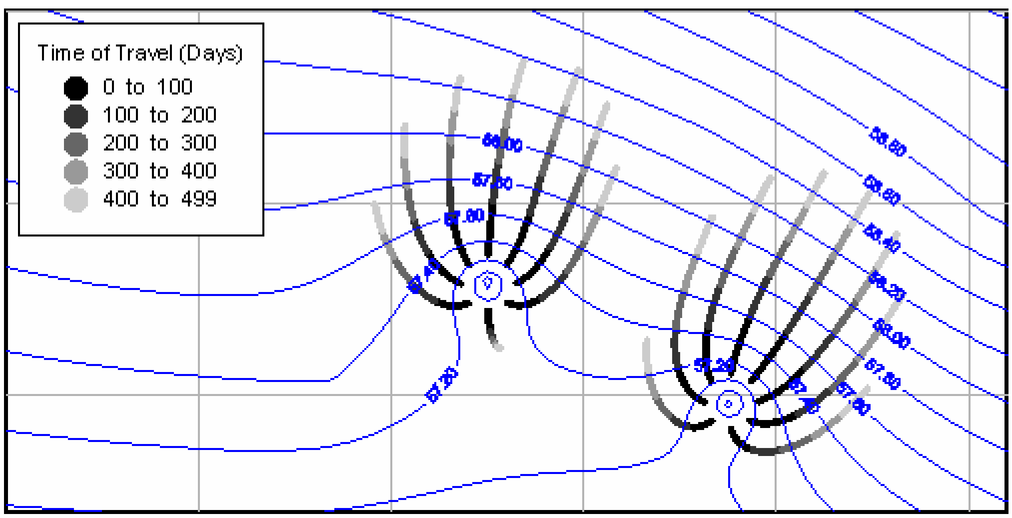
The grid values are stored in row-major order starting with the maximum coordinate. The first grid value in the grid file corresponds to the upper left corner of the map. The second grid value is the next adjacent grid node in the same row (the same Y coordinate but the next higher X coordinate).

Attachment 1

KT3D_H2O v3.0
A Program for Kriging Water Level Data using Hydrologic Drift Terms
Theoretical Documentation

KT3D_H2O v3.0

A Program for Kriging Water Level Data using Hydrologic Drift Terms



Theoretical Documentation

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& Associates, Inc.

DESCRIPTION OF THE KT3D_H2O PROGRAM SUITE

Outline

This document describes the KT3D_H2O v2.0 programs which provide a customized version of the popular kriging program KT3D (Deutsch and Journel, 1992) that has been modified to include drift terms derived from the hydrologic sciences. These drift terms are included in order to account for the influence of point, line and circular boundaries such as wells, trenches, rivers and ponds, when kriging groundwater level data. Use of the KT3D_H2O programs should always be accompanied by review of the documentation for KT3D provided in the GSLIB book (Deutsch and Journel, 1992).

Background

Though kriging is widely used for constructing gridded datasets suitable for contouring, when kriging water levels in the vicinity of pumping wells, rivers and trenches, large departures from the underlying trend are evident that correlate with areas of drawdown or mounding, and that render the maps aesthetically displeasing and illustrate weaknesses in the interpretation of the data. The methods incorporated in the KT3D_H2O programs mitigate some of these weaknesses, by including information in the kriging process to account for these features. This information is included through the description of an assumed underlying trend in the data. In this document the term drift is used synonymously with the term trend, to describe a pattern that has a deterministic source or can be approximated by deterministic means. Since the method is based on automated gridding, it can be more consistent between data sets and between analysts than methods based on hand contouring. Since the method is based on Universal Kriging, a brief overview of Universal Kriging is provided first.

Universal Kriging

Kriging is employed in the hydrologic disciplines for interpolating measured data to regular grids suitable for contouring. One advantage of kriging over other interpolation methods is that, in the absence of measurement error or replicates (co-located data), it is an exact interpolator. Chiles and Delfiner (1999) provide a detailed summary of kriging.

Two popular forms of kriging employed for interpolating real-valued data are (1) simple kriging and (2) ordinary kriging. In simple kriging, the mean of the data, m, is assumed to be constant everywhere and its value known a-priori. In ordinary kriging the mean is assumed to be unknown a-priori, and is estimated using either all or some local (moving) neighborhood of the measured data. The methods described in this discussion are based upon ordinary kriging. In the most common implementation of ordinary kriging, the mean is assumed to be constant and equivalent to the mean of the data – that is, $m = m(\mathrm{x})$. However, ordinary kriging can support a spatially varying mean which is commonly described as a smoothly-varying mean or “drift.” When a spatially varying mean is incorporated, the kriging estimate can be illustrated as the sum of two components, the mean and a zero-mean residual:

$$H(x) = m(x) + \varepsilon(x) \quad (1)$$

Where:

$H(x)$ = the kriging estimate
$m(x)$ = the smoothly-varying trend or drift
$\varepsilon(x)$ = the zero-mean random residual from the drift

This approach is commonly referred to as Universal Kriging (UK). This trend is usually a simple function of the spatial coordinates, such as a linear or quadratic function of the data X and Y coordinates. However, the kriging formulism is not limited to this form of drift, and is generally only limited to drift functions that can be fit through the solution of the (linear) system of kriging equations. For discussion on the use of trends in kriging refer to Volpi and Gambolatti (1978).

Kriging with a linear trend model or drift is available through popular programs such as Surfer® and TecPlot®. A linear drift is suitable in situations where unidirectional regional groundwater flow exists, a condition often encountered. The UK estimator for gridding water level data using this approach can be illustrated as:

$$H(x,y) = A + BX + CY + \varepsilon(x,y) \quad (2)$$

Where:

$H(x,y)$ = the estimated elevation at location (X,Y)
X = the easting or X ordinate
Y = the northing or Y ordinate
A, B, C = coefficients for the plane fitting the groundwater heads
$\varepsilon(x,y)$ = the residual from the drift

The linear drift may not be suitable in areas (a) where singularities occur within the data field such as created by pumping wells, (b) where lateral hydrologic boundaries such as the lateral termination of aquifer materials are present, (c) where there is a significant vertical component of flow, and/or (d) where there are substantial changes in aquifer properties or preferential pathways. If these effects can be represented in the trend using appropriate functions with linear coefficients, these difficulties can be resolved and kriging can produce suitable maps. Tonkin and Larson (2002) and Brochu and Marcotte (2003) describe the incorporation of analytic elements within the kriging method to account for effects due to pumped wells and boundaries.

By way of example: when kriging water level data in the presence of significant groundwater extraction or injection, the residuals (the difference between the measured data and the fitted drift surface) arising from the use of a linear drift typically indicate large local departures from the drift in the vicinity of the wells that correlate with areas of drawdown (or mounding in the case of injection wells). The use of drift terms in universal kriging based on hydrologic principals – such as drawdown in response to pumping – can improve the inference that can be drawn from measured water level data. This is illustrated in plan (Figure 1) and cross-section views (Figure 2). This is because the component of spatial correlation in the water levels that results from the influence of the boundary is explicitly included in the drift. Hence residuals are typically smaller when an appropriate drift is used. This ensures that a smaller proportion of the spatial covariance (or correlation) must be explained through the use of a variogram, the proper estimation of which might require much more data than are available. The incorporation of drift terms based on hydrologic principles is described in Tonkin and Larson (2002) and Brochu and Marcotte (2003).

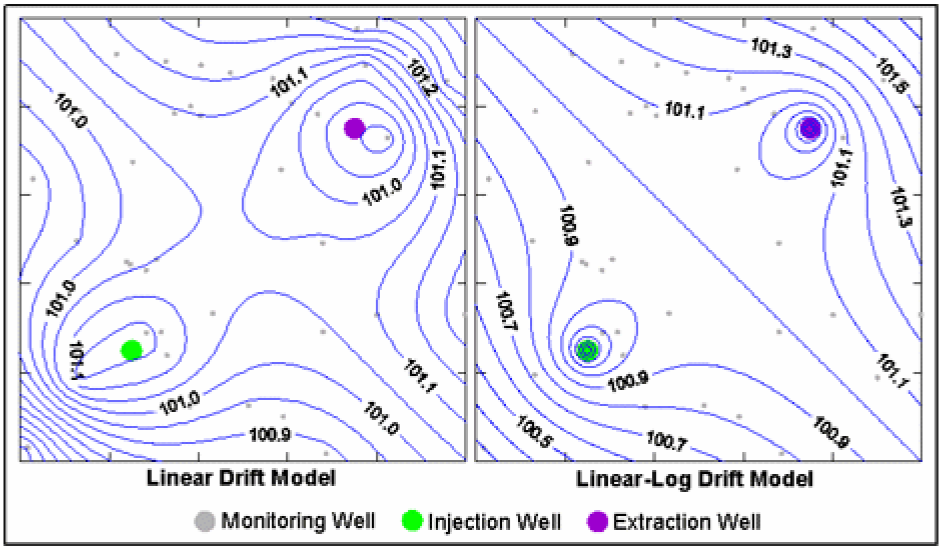


Figure 1 Plan View Comparison of Water Levels Kriged Excluding and Including Pumping Well Drift Term

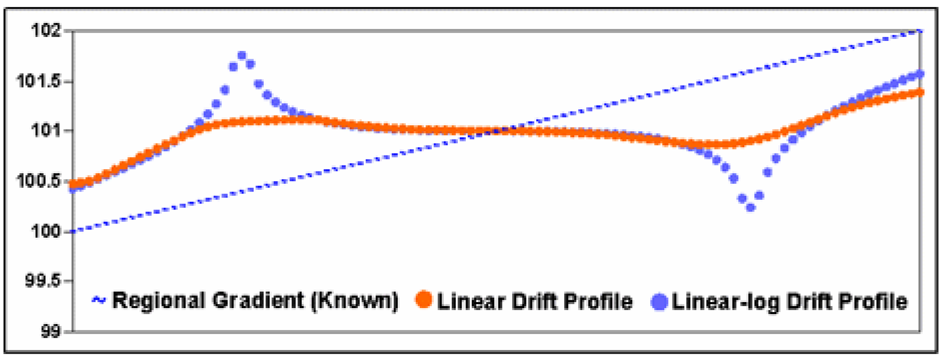


Figure 2 Section View of Water Levels from Above Kriging Example

GSLIB

GSLIB is an acronym for Geostatistical Software LIBrary, referring to a collection of geo-statistical programs developed at Stanford University. One of these programs is KT3D, a general program for point or block kriging in two or three dimensions. The GSLIB programs are fully described in Deutsch and Journel (1998). KT3D_H2O is based upon KT3D. It is strongly recommended that users of the KT3D_H2O programs obtain a copy of Deutsch and Journel (1998) both for the theoretical discussions of geo-statistics provided therein, and for the detailed descriptions of the input files required and output files produced by the KT3D program. Details of these input and output files are not provided in this documentation. However, the section “KT3D_H2O Program Inputs” described additional inputs that are required, beyond the standard KT3D inputs. In particular, KT3D uses an integer array (IDRF) to indicate which drifts are to be included in the kriging. The standard KT3D IDRF array includes nine integers, for the nine drifts available. The additional drifts added to KT3D_H2O are implemented by extending this IDRF array to include – presently – 13 integers, for the nine original drifts plus four additional drifts.

No options available to KT3D have been disabled to make KT3D_H2O. Array size limitations as listed by the dimensions in the ‘KT3D.INC’ file provided with GSLIB are adhered to in compiling KT3D_H2O. Significant arrays added to KT3D_H2O in adding the kriging and particle tracking functionality are allocatable, however, and should not be exceeded unless the program encounters problems allocating the memory. KT3D_H2O is compiled in single precision to reduce memory requirements. In several tests, comparison of grids and particle tracks calculated using single precision and double precision codes showed no noticeable improvement using double precision. However, if you encounter unsatisfactory results that may be linked to precision – in particular, if you encounter problems with particle tracking that could not be improved by modifying input options - a double-precision compiled version of the code can be provided upon request.

Additional Drift Terms Implemented in KT3D_H2O

Presently, four drift terms have been added to KT3D_H2O, beyond those included in the original KT3D program. Three of these drifts are only compatible with kriging of water levels in two dimensions (2-D). One of these drifts is compatible with kriging of water levels in 3-D. The first of these drifts to be developed, the “linear-log” drift, is described first. Subsequently the additional drift terms are described. Inputs required to implement each boundary drift term are described in the section “KT3D_H2O Program Inputs”.

1. Point Sink or Source of Known Strength

This drift was added to account for mounding (or drawdown) in response to injection (or extraction) at a known rate at one or more wells. For a single well, the Thiem equation states that, for consistent units:

$$s_r = \frac{2.3Q}{2\pi T}\log_{10}\left(\frac{R}{r}\right) \quad (3)$$

Where:

r = radial distance from the pumped well
R = radius of influence
s_r = drawdown due to pumping
Q = pumping rate
T = aquifer transmissivity

Examination of (3) indicates that pumping at a single well produces a logarithmic pattern of drawdown centered on the pumping well. Under certain assumptions, superposition can be used to sum the effect of multiple extracting or injecting wells. This essential information can be distilled and combined with the linear drift shown in (2) to give:

$$H(x,y) = A + BX + CY + D\sum_{1}^{n} Q_i \log_{10}(r_i) + \varepsilon(x,y) \quad (4)$$

Where:

$Q_i \log_{10}(r_i)$ = drawdown factor due to pumping at the i^{th} well
D = the linear regression coefficient for the drawdown factors
$\sum_{1}^{n}$ = the summation from 1 to n where n = the number of pumped wells

A full derivation of (4) is given in Tonkin and Larson (2002). This drift term can be used in combination with any of the standard two-dimensional drifts included with KT3D.

2. Horizontal Line Sink or Source of Known Strength

This drift was added to account for mounding (or drawdown) in response to horizontal linear features of known extraction (injection) rate, such as interception trenches or infiltration galleries. This implementation is based on the Analytic Element Method (AEM) described by Strack (1989) and further documented and incorporated into the AEM program TWODAN (Fitts, 2004). The complex potential representing a line sink is:

$$\Omega = \frac{\sigma L}{4\pi}\left((Z+1)Ln(Z+1) - (Z-1)Ln(Z-1)\right) \quad (5)$$

$$Z = \frac{2z - (z1 + z2)}{(z2 - z1)} \quad (6)$$

Where:

L = the length of the line sink/source

Z = a dimensionless complex variable

($z1$, $z2$) are the complex coordinates of the ends of the line

$z = x + iy$ is the point where Z and Ω are evaluated

Since σL, the discharge-per-unit-length is known out the outset then solving for Ω is a linear problem that can be included in the linear kriging system of equations. This essential information can be distilled and combined with the linear and logarithmic drifts shown in (4) to give:

$$H(x,y) = A + BX + CY + D\sum_{1}^{n} Q_i \log_{10}(r_i) + E\sum_{1}^{m} L(r_i) + \varepsilon(x,y) \quad (7)$$

Where:

$L(r_i)$ = drawdown factor due to effects of the i^{th} line sink

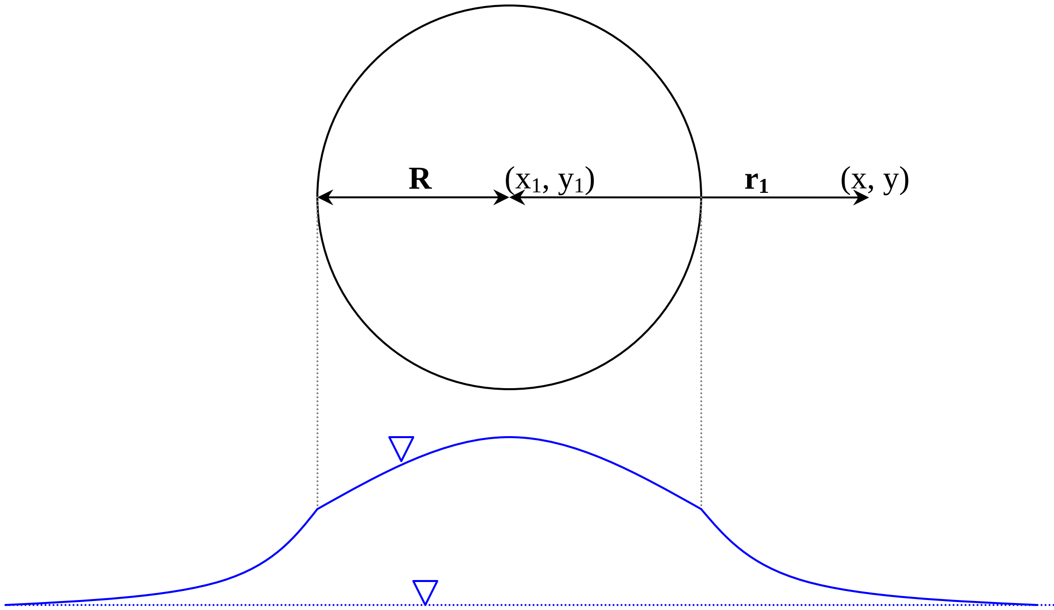
E = the linear regression coefficient for the line sink factors

$\sum_{1}^{m}$ = the summation from 1 to m where m = the number of line sinks

This drift is *only* compatible with 2-D kriging. This drift can be used in combination with the “Point Sink or Source of Known Strength”, and with any of the standard 2D drifts included with KT3D.

3. Circular Leaking Pond of Known Strength

This drift was added to account for the potentiometric response of a water table (unconfined) aquifer to infiltration through the base of a circular pond. The approach is based on the Analytic Element Method (AEM) described by Strack (1989). For a circular pond of radius R this can be represented by the following schematic and equations:



Within the element:

$(0 \leq r_1 \leq R)$ $$G_p(x, y, x_1, y_1, R) = -\frac{1}{4}\left[(x - x_1)^2 + (y - y_1)^2 + R^2\right] \quad (8)$$

Outside the element:

$(R \leq r_1 < \infty)$ $$G_p(x, y, x_1, y_1, R) = -\frac{R^2}{4} Ln \frac{(x - x_1)^2 + (y - y_1)^2}{R^2} \quad (9)$$

This essential information can be distilled and combined with the linear, logarithmic and line sink/source drifts shown in (7) to give:

$$H(x,y) = A + BX + CY + D\sum_{1}^{n} Q_i \log_{10}(r_i) + E\sum_{1}^{m} L(r_i) + F\sum_{1}^{o} P(r_i) + \varepsilon(x,y) \quad (10)$$

Where:

$P(r_i)$	= mounding factor due to effects of the i^{th} leaking pond feature
F	= the linear regression coefficient for the leaking pond features
$\sum_{1}^{o}$	= the summation from 1 to o where o = the number of pond features

This drift is *only* compatible with 2-D kriging. This drift can be used in combination with the “Point Sink or Source of Known Strength” and with the “Horizontal Line Sink or Source of Known Strength”, and with any of the standard drifts included with KT3D.

KT3D_H2O Program Inputs

This section describes the names and values of variables required in the modified KT3D ‘PAR” file, and the names and formats of new input files, that are required to implement the hydrologic drift terms and(or) the particle tracking described above. First, the variables that are required within the modified KT3D ‘PAR’ file are listed and described.

New ‘PAR’ File Variables

All additional inputs required beyond those usually supplied for kriging water level data using KT3D are now detailed.

The following entries in the ‘PAR’ file for kriging with new drift terms must be placed at the END of the 9 typical drift integers:

idrif(10) idrif(11) idrif(12)

The following entries in the ‘PAR’ file for particle tracking must be placed together on one additional line at the END of the KT3D ‘PAR’ file. These variables are only read if the particle tracking option is selected on the GUI KT3D_H2O:

iback nptp conduct porosity stepsize nparticles xprad nrads nout

Variable	**Description**
idrif(10)	If idrif(10) = 0 or is absent, no action is taken. If idrif(10) = 1 – the 2-D linear-log drift term is added. KT3D_H2O expects to find a file ‘2DWELL.DAT’ in the working directory that lists the extraction and/or injection wells. Extraction is indicated by a positive rate.
idrif(11)	If idrif(11) = 0 or is absent, no action is taken. If idrif(11) = 1 – the 2-D line sink drift term is added. KT3D_H2O expects to find a file ‘2DSINK.DAT’ in the working directory that lists the sinks/sources. Extraction is indicated by a positive pumping rate.
idrif(12)	If idrif(12) = 0 or is absent, no action is taken. If idrif(12) = 1 – the 3-D partial-penetration drift term is added. KT3D_H2O expects to find a file ‘3dwell.DAT’ in the working directory that lists the extraction

	and/or injection wells. Extraction is indicated by a positive rate.
Iback	If iback > 0 perform backward tracking If iback < 0 perform forward tracking
Nptp	The number of particle tracking steps to take
Conduct	The aquifer hydraulic conductivity in units consistent with the kriging data files
Porosity	The aquifer porosity
Stepsize	The length of the particle-tracking step
nparticles	If nparticles > 0 - the number of particles to be placed in an envelop around each well listed in the file ‘2DWELL.DAT’ and each line segment listed in the file ‘2DSINK.DAT’. Note multiple envelopes can be defined (see nrads) If nparticles < 0 - KT3D_H2O expects to find a file ‘PTRACK.IN’ in the working directory that lists particle starting locations
xprad	The radius of the innermost envelop of particles around each well listed in ‘2DWELL.DAT’ and each line segment listed in the file ‘2DSINK.DAT’. This only applies where nparticles > 0.
Nrads	The number of envelopes of particles around each well listed in ‘2DWELL.DAT’ and each line segment listed in the file ‘2DSINK.DAT’. This only applies where nparticles > 0. The radius of each envelop is a multiple of the radius of the inner envelop (xprad)
Nout	The frequency with which to report particle locations to the output file ‘PTRACK.OUT’. Locations are only written when the calculation step is a multiple of nout. This keeps file sizes smaller.

Point Sink or Source of Known Strength

In order to execute the KT3D_H2O linear-log approach to kriging for a 2-D water level data set, given a KT3D input (‘PAR’) data set, the following steps are required:

- Construct an accessory file (*2DWELL.DAT*) that contains information required to define the well location(s) and extraction injection rate(s). The format of this file is shown below.
- Change the tenth drift term in the ‘PAR’ file from 0 to 1.
- Use the modified KT3D_H2O program.

Format of file “2DWELL.DAT”

n	Number of wells
X(i), Y(i), Q(i), QT(i)	X, Y coordinates, rate, type for first well
………………	……

X(n), Y(n), Q(n), QT(n) X, Y coordinates, rate, type for last well

The purpose of QTYPE is to indicate if the well is considered a “Recovery Well” (QTYPE = “R”) for which it is necessary to map and illustrate particle capture; or a “non-Recovery Well” (QTYPE = “NR”) at which particles may be recovered, but for which it is not necessary to map and illustrate particle capture.

Horizontal Line Sink or Source of Known Strength

In order to execute the KT3D_H2O horizontal line sink or source of known strength, given a KT3D input (‘PAR’) data set the following steps are required:

- Construct an accessory file (*2DSINK.DAT*) that contains information required to define the line sink/sources including the segment location(s) and extracion/injection rate(s). The format of this file is shown below.
- Change the eleventh drift term in the ‘PAR’ file from 0 to 1.
- Use the modified KT3D_H2O program.

Note that the rate, or strength, of the line segment is specified in terms of rate-per-unit-length. For example, a 10 foot segment with a total extraction of 10 gpm has a rate (strength) of 1.0 (gpm/ft).

The format of the file “2DSINK.DAT” depends on the method being used to define the line sinks. If line sinks are isolated in space, then NLIN must be > 0, and the start and end of each line segment must be specified. In this case, there will be NLIN x 2 entries in the file. If line sinks are connected at their ends, then the user can opt to only list the points that define the total line. In this case, the number of actual line segments will be (NLIN x 2 – 1), and the start of each subsequent segment is identified by KT3D_H2O as the end of the previous segment. Note that presently this option can only be used if every segment is of equal strength-per-unit-length (this is not a limitation of the method).

Format of file “2DSINK.DAT” *if NLIN>0*

nlin	Number of line segments
lxs(i),lys(i),li(i),lv(i)	X-start, Y-start, flag, rate for first segment

lxe(i),lye(i),li(i),lv(i)	X-end, Y-end, flag, rate for first segment
…………………………	……
lxs(nlin),lys(nlin),li(nlin),lv(nlin)	X-start, Y-start, flag, rate for last segment
lxe(nlin),lye(nlin),li(nlin),lv(nlin)	X-end, Y-end, flag, rate for last segment

Format of file “2DSINK.DAT” *if NLIN<0*

nlin	number of line segments = nlin x 2 – 1
lxs(i),lys(i),lind(i),lval(i)	X-start, Y-start, flag, rate for first segment
……….	……….
lxe(nlin),lye(nlin),li(nlin),lv(nlin)	X-end, Y-end, flag, rate for last segment

Example Data Sets

[Note: examples to be converted to be used in KT3D_H2O GUI Version 3.0]

Point Sink or Source of Known Strength

The KT3D_H2O suite of programs is supplied together with an example multiple-pumping-well data set, as described in the paper by Tonkin and Larson (2002), and output files in Surfer™ format (“Verification-2DWells.srf “) showing the resulting water-level surface and example particle tracks. Since these results are provided in Tonkin and Larson (2002) they are not included in this documentation. This example data set includes five extraction wells and backward particle tracking using 1 concentric circle of particles placed around each well (this example data set is provided with the program). The first table shows the entries in the kriging input (‘PAR’) file; the second table shows the entries in the pumping data file ‘2DWELL.DAT’.

```
              Parameters for KT3D_H2O
              ****************************

START OF PARAMETERS:
test.dat                         \ file with data
1   2   0    3    0              \    columns for X, Y, Z, var, sec var
-1.0e21   1.0e21                 \    trimming limits
0                                \ option: 0=grid, 1=cross, 2=jackknife
none.dat                         \ file with jackknife data
1   2   0    3    0              \    columns for X,Y,Z,vr and sec var
0                                \ debugging level: 0,1,2,3
KT3D.dbg                          \ file for debugging output
KT3D.out                          \ file for kriged output
201 857000 25                    \ nx,xmn,xsiz
251 238000 25                    \ ny,ymn,ysiz
1    1     1                     \ nz,zmn,zsiz
1    1     1                     \ x,y and z block discretization
30   40                          \ min, max data for kriging
0                                \ max per octant (0-> not used)
20000.0  20000.0  20.0           \ maximum search radii
 0.0   0.0   0.0                 \ angles for search ellipsoid
1  0.0                           \ 0=SK,1=OK,2=non-st SK,3=exdrift
1 1 0 0 0 0 0 0 0 1 0 0          \ drift: x,y,z,xx,yy,zz,xy,xz,zy,Q,L,PP
0                                \ 0, variable; 1, estimate trend
none.dat                         \ gridded file with drift/mean
```

```
4                                    \    column number in gridded file
1    0.0                             \ nst, nugget effect
1    1.0  0.0   0.0   0.0            \ it,cc,ang1,ang2,ang3
      20000.0 20000.0 20.0           \    a_hmax, a_hmin, a_vert
1 500 100. 0.2 1.0 8 50. 1 5         \ tracking: iback,nptp,hydcond,porosity,stepsize,nparticles,xprad,nrads,nout
1.e-4 1.e-10  0.80  1.e-6  1.e-3  \roerr,tiny,safety,eps,vsmall

#note - the code knows if particle tracking has been selected by an integer flag passed
#from the VB GUI to the KT3D_H2O DLL
```

```
5
858951  242823  43316  R
859806  239179  43315  R
857654  241948  52941  R
859752  241291  43316  R
860383  240985  48128  R
```

Horizontal Line Sink or Source of Known Strength

The KT3D_H2O suite of programs is supplied together with an example multiple-line sink/source data set and output files in Surfer™ format ("Verification-2DSink.srf ") showing the resulting water-level surface and example particle tracks. This example data set includes two line sinks (this example data set provided with the program). The first

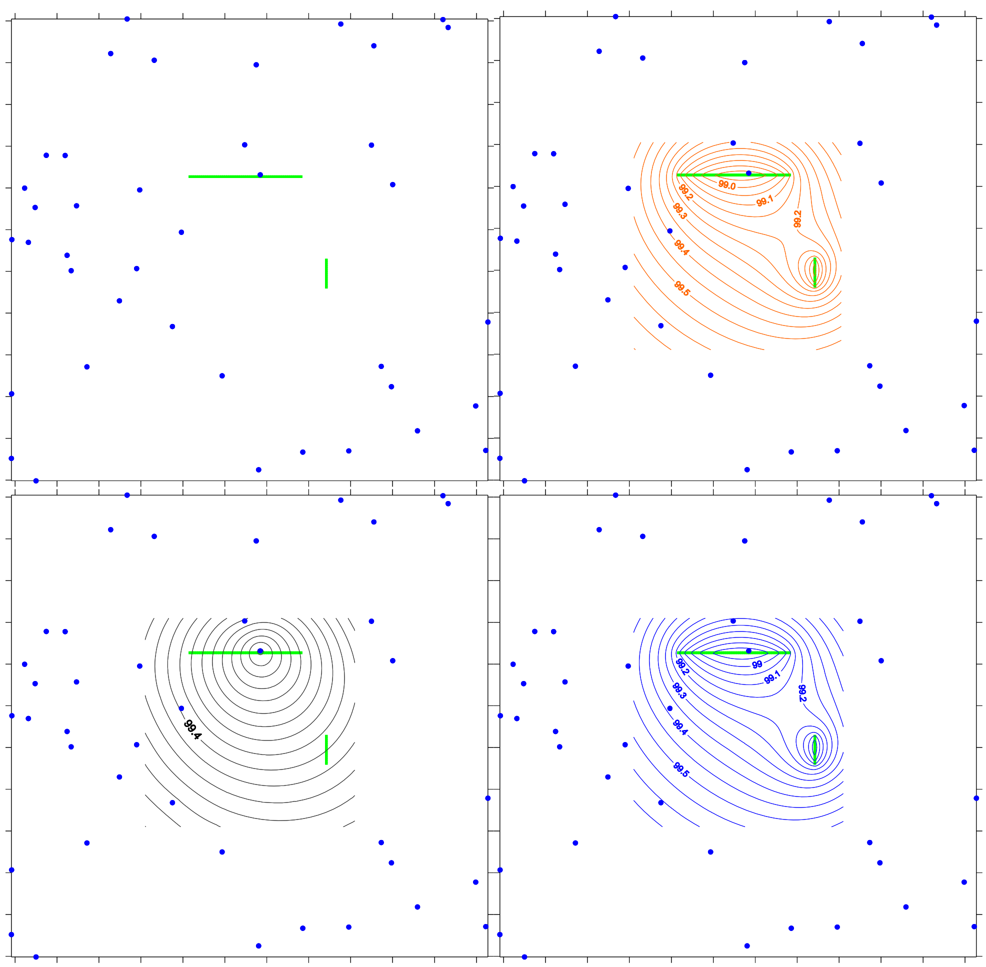


Figure 5 2D Sink of Known Strength: (i) Sinks, (ii) MODFLOW, (iii) Ordinary Kriging (no Sink Drift) (iv) 2D Sink Drift. Blue – monitoring locations.

table shows the entries in the kriging input ('PAR') file; the second table shows the entries in the line segment file '2DSINK.DAT'. Images from the results are provided as Figure 5. The slight discrepancy between the MODFLOW model and KT3d_H2O results is due to the MODFLOW discretization and the proximity of the constant head boundary.

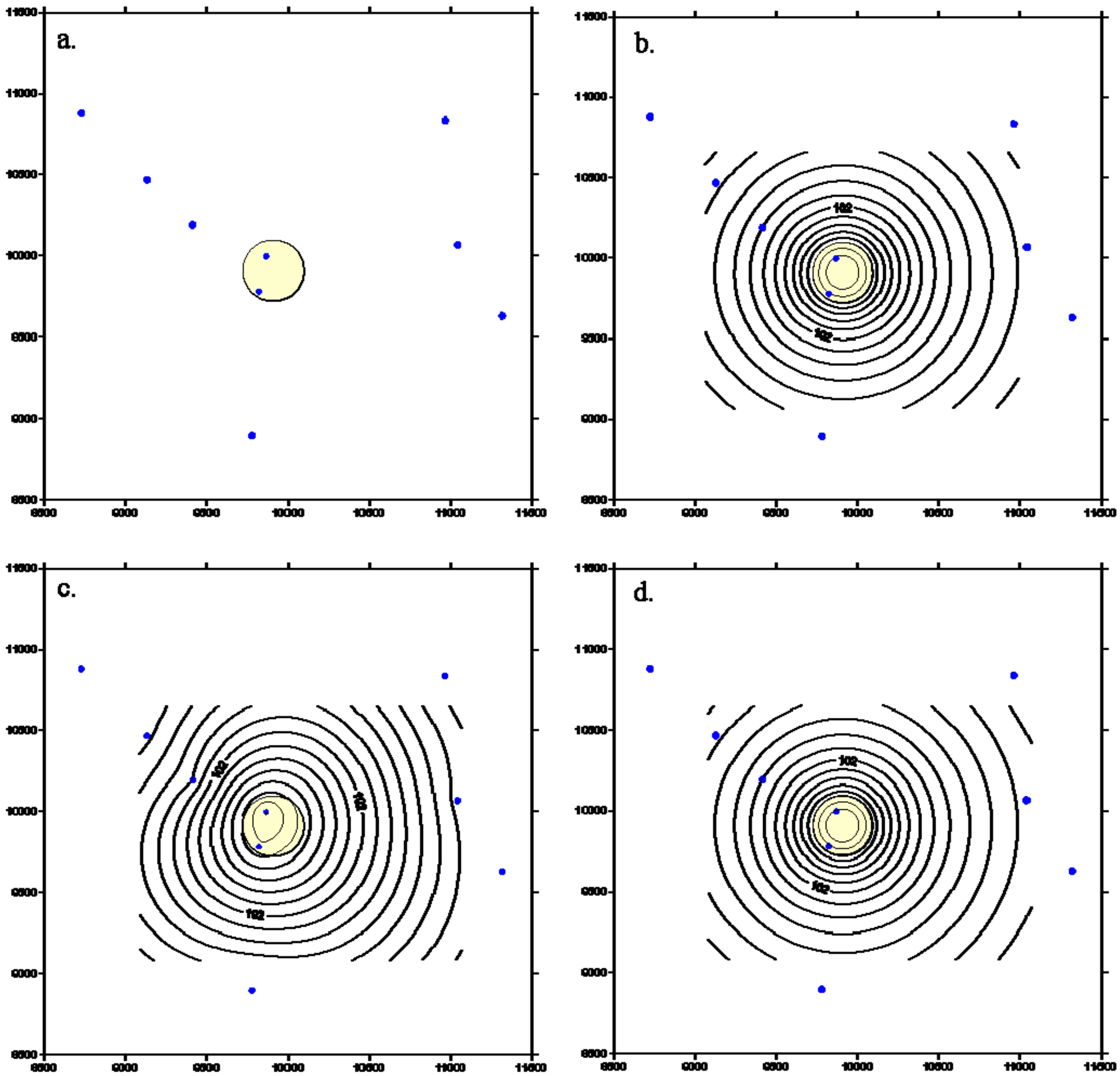
```
                Parameters for KT3D
                *******************

START OF PARAMETERS:
wl-2DSINK.DAT                        \ file with data
1   2   0    3    0                  \   columns for X, Y, Z, var, sec var
-1.0e21   1.0e21                     \   trimming limits
0                                    \ option: 0=grid, 1=cross, 2=jackknife
none.dat                             \ file with jackknife data
1   2   0    3    0                  \  columns for X,Y,Z,vr and sec var
0                                    \ debugging level: 0,1,2,3
kt3d.dbg                             \ file for debugging output
kt3d.out                             \ file for kriged output
101 6100.01 50                       \ nx,xmn,xsiz
101 6100.01 50                       \ ny,ymn,ysiz
1    1      1                        \ nz,zmn,zsiz
1    1      1                        \ x,y and z block discretization
40   40                              \ min, max data for kriging
0                                    \ max per octant (0-> not used)
20000.0  20000.0  1.0                \ maximum search radii
0.0   0.0   0.0                      \ angles for search ellipsoid
1  0.0                               \ 0=SK,1=OK,2=non-st SK,3=exdrift
1 1 0 0 0 0 0 0 0 0 1 0              \ drift: x,y,z,xx,yy,zz,xy,xz,zy,Q,R,PP
1                                    \ 0, variable; 1, estimate trend
none.dat                             \ gridded file with drift/mean
4                                    \   column number in gridded file
1    0.0                             \ nst, nugget effect
1    5.0  0.0   0.0  0.0             \ it,cc,ang1,ang2,ang3
     15000.0 15000.0 1.0             \ a_hmax, a_hmin, a_vert
1 100 100. 0.2 1.0 -1 50. 1      \ tracking: iback,nptp,hydcond,porosity,stepsize,nparticles,xprad,nrads
1.e-4 1.e-10  0.80  1.e-6  1.e-3  \roerr,tiny,safety,eps,vsmall
#note - the code knows if particle tracking has been selected by an integer flag passed
#from the VB GUI to the KT3D_H2O DLL
```

```
2
7145.00  10270.00   1 -38.6
9845.00  10270.00   1 -38.6
10420.00  7595.00   1 -75
10420.00  8295.00   1 –75
```

Circular Leaking Pond of Known Strength

Example data including water elevations and pond drift parameters are listed in the tables below. Output files showing the resulting water-level surface are supplied in Surfer™ format (“CircDriftEx.srf“). Images from the results are shown here.



Circular leaking pond of known strength: (a) Pond with known infiltration rate, (b) MODFLOW, (c) Ordinary kriging with no pond drift, (d) Kriging with pond drift. Blue points indicate monitoring locations.

Data Used for Verification of KT3D_H20 Circular Pond Drift			
X	Y	Head	Well Name
7583	10691	100.887305	T1
8339	7422	100.774772	T2
10858	8022	100.981328	T3
9867	9993	102.713499	T4
11041	10067	101.36511	T5
7641	9718	100.935022	T6
7996	9174	101.00069	T7
8721	10879	101.181256	T8
9821	9777	102.583003	T9
12196	8674	100.851355	T10
9814	11990	100.989186	T11
10704	8420	101.121289	T12
11320	9630	101.221638	T13
9064	7512	100.866058	T14
10962	10836	101.236196	T15
9411	10192	101.797811	T16
11220	7977	100.91872	T17
11713	10338	101.062477	T18
9775	8894	101.435422	T19
9125	10467	101.472925	T20

Drift Parameters Used for Verification of KT3D_H20 Circular Pond Drift				
X	Y	Radius	Strength	Drift Term
10000	10000	186	0.1	1

Acknowledgements

We offer sincere gratitude to Charles Fitts, of Fitts Solutions, ME, for his invaluable guidance when we encountered difficulties programming the line sink/source. The correspondence that successfully led to the inclusion of this drift term helped greatly with our understanding of the Analytic Element Method.

Technical Support

Limited technical support can be obtained by writing to matt@sspa.com.

Frequently Asked Questions

How can I make a map of my 'best-fit' drift (trend) surface, assuming that the errors in the measurement data are uncorrelated, just to see a map of it?

This is analogous to performing a least-squares fit of the function:

$$Z = A + BX + CY + D(Q) + E(L) + F(P) + \varepsilon$$

… where A, B, C, D, E and F are drift coefficients; X,Y are Cartesian coordinates; Q is the 2-D well drift component summation; L is the known strength line sink/source drift component summation; P is the known strength circular elements drift component summation. The error term (i.e. residual) is not included - the gridded surface will not be an exact interpolator but will be the best fit of the trend. Theoretically, fitting of this surface is achieved using a horizontal ('pure nugget') variogram. With the code provided, this is achieved by setting the variogram parameters a_hmin, a_hmax, a_vert to 0.1, 0.1, 0.1, and setting the trend variable to 1 ('estimate trend').

Should I include water levels measured in extraction wells in the observed water level data set?

Since the linear-log drift accounts for the effects of extraction or injection, water levels measured in extraction wells should in general **not** be used as observations. The kriging code as currently written does not account for linear/non-linear well losses at extraction wells, and hence the drift coefficients (and map) will be biased by these effects, if in fact a division-by-zero error is not encountered first (see below). There are plans to add an additional drift term to account for linear well losses during the kriging as an additional drift term. Please write to matt@sspa.com if you feel this drift term would be valuable to your needs.

The code reports a division-by-zero error upon execution.

Check that none of your extraction/injection wells and observation (monitoring) wells are collocated – i.e. have the same X and Y coordinates. This will cause a division-by-zero error in the estimation of the drift terms since the separation distance is zero. The current version of the kriging program checks for co-located wells and should identify these and terminate with an error message.

The code reports NAN (the Fortran 'not-a-number' flag) for an estimation point and/or for a lagrange multiplier.

Check that none of your estimation points - i.e. a node point for which we were asking the code to give an estimate - and observation (monitoring) wells are collocated – i.e. have the same X and Y coordinates. This *may* cause an error in estimating the kriging weights under some circumstances since the separation distance is zero. The current version of the kriging program checks for co-located wells and should identify these and terminate with an error message reporting the conflict(s).

NOTE: Every effort should be made to ensure there are no collocation conflicts - either extraction wells at the same location as observation wells or observation wells at the same location as an estimation point. This can be done in one of two ways - (1) the user should check these conflicts will not occur; (2) by pragmatically by simply adding some small delta-d to the observation well location coordinates. The latter, pragmatic approach of adding some delta-d value to the X or Y of the observation points should in the majority of instances avoid these conflicts without affecting results or their interpretation however the magnitude of the value delta-d will be case specific.

I get a division-by-zero error, but have checked all my data and have no collocated wells or points.

This can occur where, for example, the data set contains one extraction well, and one injection well, and these wells form a recirculation system with extraction equaling injection. This can be pragmatically overcome by adding a small delta-q to one of the wells. Again, this is a pragmatic solution, and delta-q is case-specific.

Notes on an Arbitrary 2-D Polyline Boundary

A drift was incorporated in KT3D_H2O at one time to provide a general method for representing fairly distant rivers and other extended length features. This approach is not as rigorously founded as the drifts described in this document. The drift was derived on the basis of an infinite, fully penetrating line sink:

- in a confined aquifer there is no curvature of the water table and the slope towards the boundary feature is planar
- in an unconfined aquifer with no recharge the curvature of the water table approximates a quadratic.

This form of drift term is implemented as:

$$h_{ij} = \left(\frac{1}{a}\right) r^{p} + h_R$$

Where h_{ij} is the elevation of the potentiometric surface at location (i,j); a is a scalar that is a function of T, recharge, and aquifer type; p is a power term which is typically specified as 0.5 but is a function of the penetration of the feature; r is the distance of location (i,j) from the boundary feature; and h_R is the elevation of the boundary feature. The user can provide an arbitrary power for the drift ranging from 1.0 (i.e., linear) approximating the simple confined case, to 0.5 (i.e., quadratic) approximating the second case. Note that the drift does not presently account for a slope in this feature – e.g., a bed slope in a river across the data domain. *NOTE: In the current version of KT3D_H2O this drift term is disabled. Please contact matt@sspa.com if this drift may suite your needs.*

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Appendix A: Kriging Water Levels with a Regional-linear and Point-logarithmic Drift, Ground Water, 2002

Kriging Water Levels with a Regional-Linear and Point-Logarithmic Drift

by Matthew J. Tonkin[1] and Steven P. Larson[1]

Abstract

Ground water levels measured in the vicinity of pumping wells are kriged using a regional-linear and point-logarithmic drift, the latter derived from the approximation to the Theis equation for drawdown in response to a pumping well. Kriging is widely used throughout the hydrogeologic discipline, most commonly as the preferred method for constructing gridded hydrogeologic datasets suitable for contouring. Residuals arising from using the most common (linear) drift to krige water levels in the vicinity of extraction wells often indicate large local departures from the linear drift, which correlate with areas of drawdown. The combined regional-linear and point-logarithmic drift accounts for these drawdowns using a logarithmic approximation for the curvature of the potentiometric surface. The drift model approximates the principal physical processes that govern ground water flow and ultimately govern the autocorrelation of ground water elevation data. This approach produces maps of contoured water levels that more realistically represent physical conditions and allow for improved interpretation of measured water-level data by including features and information known to be present. Additional benefits include an improved estimate of the regional (background) hydraulic gradient and generation of an approximately flow-conserved grid suitable for two-dimensional particle tracking.

Introduction

Kriging is widely used throughout the hydrogeologic discipline as the preferred method for constructing gridded hydrogeologic datasets suitable for contouring. Kriging was introduced as a least-squares estimator that improved on methods such as distance weighting or polynomial interpolation for which weighting was a determinant (Delhomme 1978). An advantage of kriging is that, in the absence of measurement error, it is an exact interpolator at measurement points. In addition, kriging yields both estimated values and estimate variances (Skrivan and Karlinger 1977). Kriging is ideally an investigative and iterative process, including development and fitting of an analytical function representing the underlying trend or drift where evidence exists for such, and development of a semivariogram to describe the pattern of residuals (measured data minus drift) (Volpi and Gambolati 1978). This universal kriging approach is not typically adopted for gridding ground water level data. Despite the extensive literature that discusses kriging, calculating custom drift functions is not a straightforward matter, and standard approaches rarely extend beyond linear and polynomial drift models (Chiles and Delfiner 1999). In areas of fairly uniform regional hydraulic gradients, the linear drift can improve the aesthetics of a contour map. However, visual inspection of contours generated in this manner indicates that the linear drift does not produce a surface that is adequately close to conserving flow in areas of localized discharge or recharge.

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As a consequence, interpretation of water levels constructed without a drift model or using a linear drift is typically limited to broad features, such as principal direction(s) of flow and areas of significant drawdown or mounding. Although this capability can be improved by increasing the number and density of monitoring wells—provided the wells are suitably located—water-level monitoring budgets rarely allow for a network sufficient for accurately representing the curvature of the potentiometric surface near extraction wells. Such a network is particularly important in downgradient areas where constraint of the capture zone by determination of the stagnation zone can be critical. All of these factors make contouring of measured ground water elevations typically unsuitable for delimiting the capture zone of a pumping well.

An approach for gridding ground water level data is presented here. Application of this method produces contoured data maps that can improve interpretation of measured water-level data. A combined regional-linear and point-logarithmic drift is employed to specifically account for drawdown and mounding in the vicinity of extraction and injection wells using a logarithmic approximation for the curvature of the potentiometric surface. The point-logarithmic drift is derived from the approximation to the Theis equation for drawdown due to a pumping well. Examples are provided comparing contoured ground water levels measured in the vicinity of pumping wells, kriged using no-drift, linear-drift, and the new combined drift models. Data requirements for the new method are limited to knowledge of pumping activities, including location and rates, and knowledge of the geographic coordinates of monitoring wells. Primary benefits from application of this method include improved estimates of the regional (background) hydraulic gradient and generation of a gridded dataset suitable for two-dimensional particle tracking.

Inclusion of a logarithmic component in the drift model for kriging water-level data has been previously proposed but, to our knowledge, not presented (Volpi and Gambolati 1978). The approach presented here arose without knowledge of this prior study and, it is hoped, complements and extends the discussion presented therein with some examples.

Drift Model

Kriging using a drift or trend model, termed "universal kriging," is typically performed where a smoothly varying trend is present in the data. The drift component is usually modeled as a function of the data coordinates, whose unknown parameters are fitted from the data (Deutsch and Journel 1998). The underlying model is then the sum of the drift component plus the residuals:

$$Z(u) = m(u) + R(u) \qquad (1)$$

where

- $Z(u)$ = value of random or regionalized variable
- $m(u)$ = drift (trend)
- $R(u)$ = residual component
- u = Cartesian coordinate location (x,y) for two-dimensional kriging.

The residual component is typically modeled as a zero-mean stationary random function (RF) (Deutsch and Journel 1998).

A linear drift is defined as the least-squares fit of the planar surface, described by

$$\text{Linear drift} = A + BX + CY \qquad (2)$$

where X is x (or easterly) coordinate (dimension of length [L]); Y is y (or northerly) coordinate (L); and A, B, and C are fitted parameters of the drift model calculated from the data.

The kriging algorithm identifies the least-squares fit of the drift model to the data, assuming that residuals R(u) are uncorrelated (Deutsch and Journel 1998).

The Theis equation for drawdown in response to pumping can be approximated using (Ferris et al. 1962; Rouse 1949)

$$s = \frac{Q}{4\pi T}\ln\left(\frac{2.25Tt}{r^2S}\right) \qquad (3)$$

where

- Q = pumping rate at extraction well (L^3T^{-1})
- S = aquifer storage (−)
- T = aquifer transmissivity (L^2T^{-1})
- s = drawdown of the potentiometric surface (L)
- r = radial distance to the pumping well (L)
- t = time since pumping began (T)
- π = ~ 3.14159
- ln = natural logarithm.

Equation 3 describes a logarithmic cone of depression, centered on the extraction well. This can be rewritten as

$$s = \frac{Q}{4\pi T}\left[\ln\left(\frac{2.25Tt}{S}\right) + \ln\left(\frac{1}{r}\right)^2\right] = \frac{Q}{4\pi T}\left[\ln\left(\frac{2.25Tt}{S}\right) + 2\ln\left(\frac{1}{r}\right)\right] \qquad (4)$$

At any time when the change in hydraulic gradients is zero, the first term in Equation 4 can be considered a constant, and the drawdown at a monitoring well is inversely proportional to the logarithm of the radial distance of the monitoring well from the extraction well, proportional to the pumping rate Q and inversely proportional to the transmissivity (T). Combining Equations 2 and 4, the drift (termed "linear-log" in the following discussion) is described by

$$\text{Drift}_{ij} = A + BX + CY - \frac{Q}{2\pi T}\ln(r) \qquad (5)$$

Because the transmissivity is assumed constant throughout the aquifer, the relative magnitude of drawdown at a monitoring well due to pumping at multiple extraction wells is determined only by Q and r. Using the principle of superposition, the drawdown due to pumping of up to n extraction or injection wells can be summed, i.e.,

$$s_{ij} = -\sum_{1}^{n} Q_n \ln(r_n) \qquad (6)$$

Where s_{ij} is the drawdown at location (i, j)(L); Q_n is the pumping rate at the nth extraction well (L^3T^{-1}); r_n is the radial distance of extraction well Q_n from location (i, j)(L); and (i, j) may represent (row, column) grid location or Cartesian coordinates.

The complete linear-log drift is then invoked in the kriging routine as

$$\text{Drift}_{ij} = A + BX + CY + s_{ij} \qquad (7)$$

By including the logarithmic component, the drift model approximates the principal physical processes that govern ground

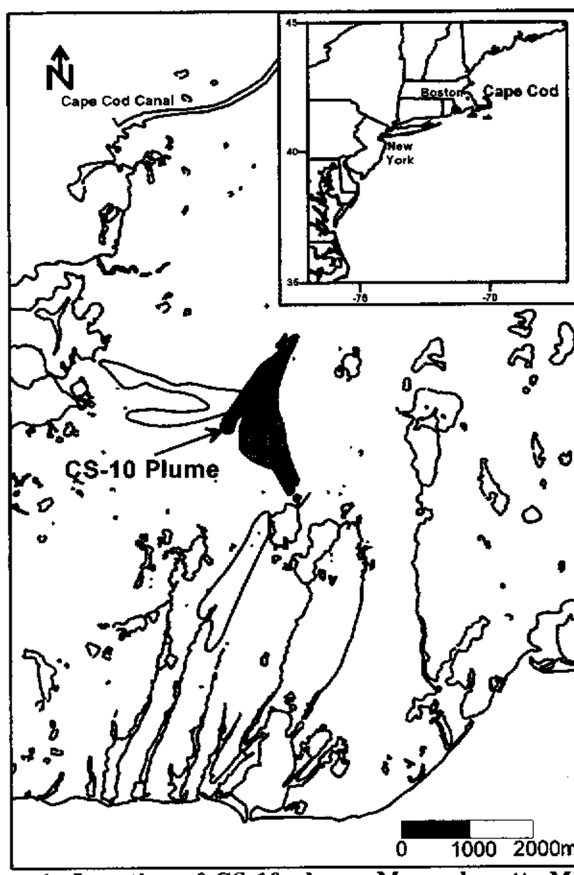

Figure 1. Location of CS-10 plume, Massachusetts Military Reservation, Cape Cod.

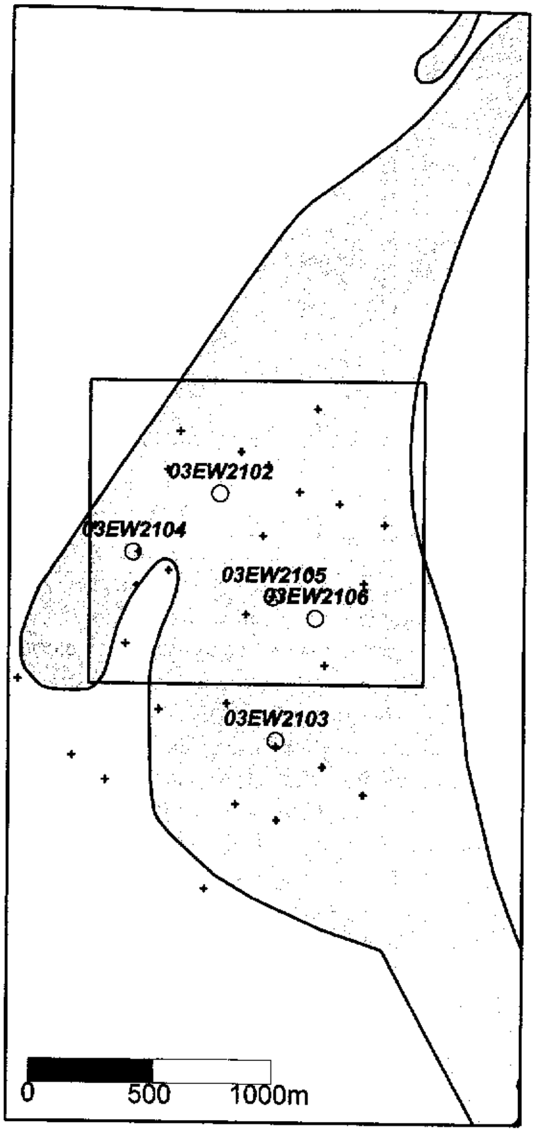

Figure 2. Location of monitoring and extraction wells of the CS-10 plume, and the local area of well-capture estimation.

water flow and ultimately govern the autocorrelation of ground water elevation data. Accordingly, assumptions underlying the Theis equation are implicit in the kriging routine, principally (Rouse 1949):

- The pumping well penetrates and receives water from the entire saturated thickness of the aquifer.
- The aquifer is confined; if the aquifer is unconfined, drawdowns should be less than ~10% of the saturated thickness of the aquifer.
- The aquifer is homogeneous, isotropic, and of infinite areal extent.
- The drawdown and/or mounding has reached a steady-state condition. If this is not the case, the rate of change in hydraulic gradients should approach zero.

Because the form of the underlying drift is assumed to apply to the entire dataset, the drift model parameters are calculated from a global estimation of Z(u). Linear-log kriging is performed using a selection of Fortran routines modified from U.S. Geological Survey Program Number K603, coded by Skriven and Karlinger (1977).

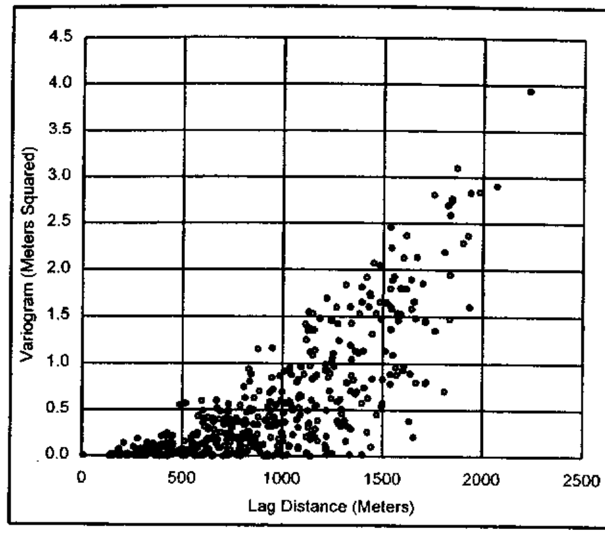

Figure 3. Measured data (raw) semivariogram.

Example Dataset: Cape Cod, Massachusetts

Water levels measured in 32 wells of the Chemical Spill-10 (CS-10) plume, Massachusetts Military Reservation (MMR), Cape Cod (Figure 1) monitoring well network were gridded using the approach detailed previously. Numerous excellent discussions of remedial activities at MMR are available in the literature, e.g., AFCEE (2000) and the MMR Web site at www.mmr.org. The principal contaminants in the CS-10 plume are trichloroethene (TCE) and perchloroethene (PCE), and the selected remedy for the plume is pump and treat. The CS-10 plume is within the Mashpee Pitted Plain (MPP) sediments, which comprise well to poorly sorted, fine- to coarse-grained sands forming a broad outwash plain that typically displays high hydraulic conductivities on the order of 2×10^{-4} m/sec (15 m/day) or greater (Hess et al. 1992). Drawdowns resulting from pumping of CS-10 extraction wells typically do not exceed 1 to 1.5 m of a total saturated thickness averaging 60 m. Assumptions underlying the Theis approximation are considered to be fairly well adhered to.

Water levels selected for this study were measured in 1999 at wells in the upgradient area of the plume, where four extraction wells were being operated to remove ground water contaminated with TCE and PCE. The monitoring network in this area is fairly dense, with monitoring well separations on the order of a few tens to a few hundred meters. Nineteen monitoring wells in the middle of the study area are shown in Figure 2; the remaining wells lie to the south and west of this local-scale map. Water-level contours are shown only for the "zoom" area because this is the area of interest for determining extraction well-capture zones. At the time water levels were collected for this study, two extraction wells had monitoring wells within 20 m for use in aquifer tests. For the remaining extraction wells, the nearest monitoring wells were ~150 m away. In the case of one extraction well (03EW2102), the water level in the nearest monitoring well was not measured, and the nearest water-level measurement was at a distance of ~300 m. The raw data semivariogram is shown in Figure 3. The parabolic behavior of the raw semivariogram is a strong diagnostic indicator of the existence of a trend in the data (Clark and Harper 2000).

Initially, point kriging was performed for a regular grid of 200×200 points, spaced on a 7×7 m grid, assuming no drift, a linear drift, and a linear-log drift. In each case, a linear semivariogram

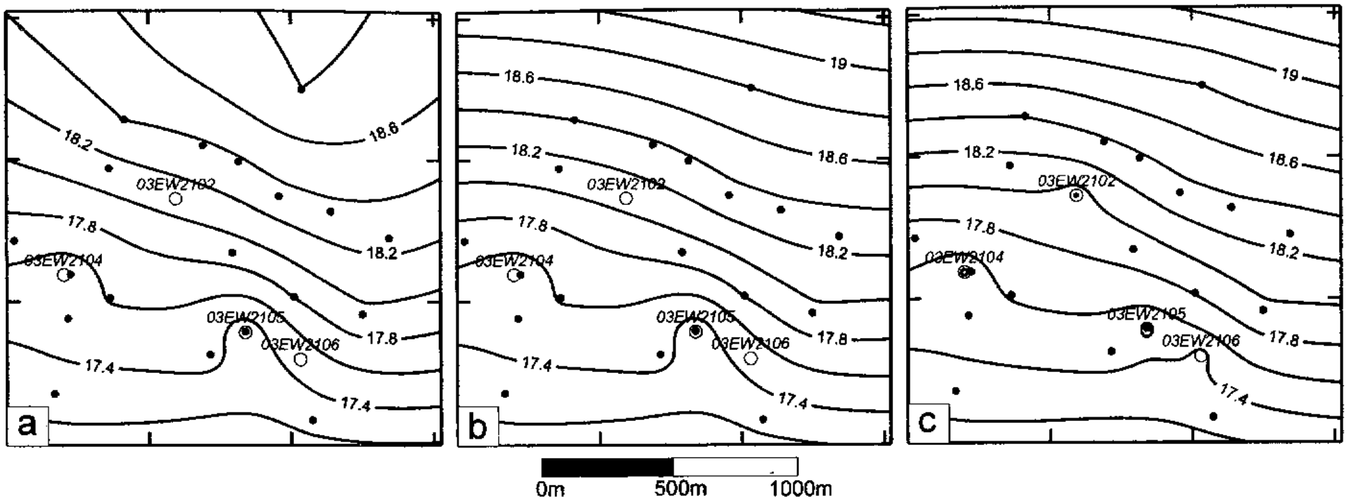

Figure 4. Comparison of ground water contours: (a) no-drift, (b) linear-drift, and (c) linear-log drift.

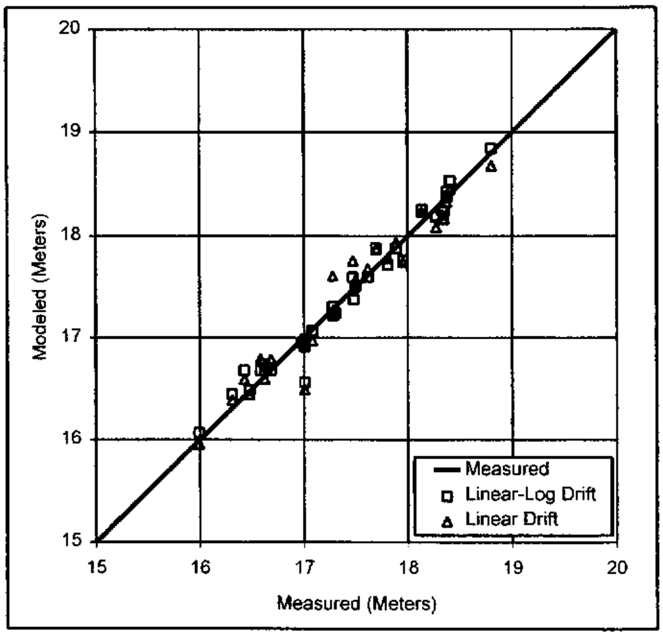

Figure 5. Calculated versus measured water level for linear and linear-log drifts.

was used. Visual comparison of the ground water contours on the three resulting maps (Figure 4) indicates:

1. In areas of high data control (closely spaced monitoring wells) and low stress (far from pumping), contours of the no-drift, the linear-drift, and linear-log maps are similar.
2. In areas of high data control (closely spaced monitoring wells) and high stress (close to pumping), the contours of the no-drift and linear-drift maps are similar; however, contours of the linear-log map exhibit the more defined structure of the underlying drift model.
3. In areas of low data control, contours of the no-drift, linear-drift, and linear-log maps differ markedly. In particular, contours of the no-drift map converge in the north of the domain where a single data point is present, resulting in an unrealistic map of the ground water surface.

As the distance from measurement points increases, the underlying drift dominates the contour pattern, and further differences between the linear and linear-log drift maps are apparent. Water-level contours constructed using the linear-log drift are concave to the extraction wells for some distance away from each extraction well. The concavity decreases with distance from each extraction well. This pattern is expected due to drawdown in response to pumping. Water-level contours calculated using the linear drift are concave close to each extraction well, but the concavity is less defined farther from the wells, and the contours display the underlying linear drift. This comparison suggests that kriging with a linear drift may result in a poor approximation of the underlying trend or regional gradient. Although the scattergrams are at first glance indistinguishable (Figure 5), on closer inspection, the linear-log drift estimates (squares) are typically closer to the line of equality than the linear-drift estimates (circles). This condition occurs largely from systematic (typically by design) bias in the location of monitoring wells close to extraction and injection wells and the tendency of the universal kriging routine to spread residuals (error) from the drift calculation throughout the gridded domain. The sum of squared differences for the two models differs by ~50%—in this case, 0.5 m^2 for the linear-log drift model and 0.78 m^2 for the linear-drift model.

The gridded ground water levels calculated with no-drift, the linear-drift, and the linear-log drift formed the basis of particle-tracking analyses using Path3D (Zheng 1992) to delineate the well-capture zones (Figure 6). The saturated thickness was simulated for a confined, single layer, isotropic homogeneous aquifer of 60 m. Comparison of the resulting maps indicates:

1. In areas of high data control and low stress (consistent gradients), particle tracks are similar.
2. In areas of high data control and a single stress (e.g., in the area of steep gradients close to 03EW2104), particle tracks of the linear and linear-log drift maps are quite similar.
3. In areas of fairly high data control and more than one stress (e.g., in the area of complex gradients close to 03EW2105 and 03EW2106), the linear and linear-log drift particle tracks differ markedly. In particular, the capture zone of 03EW2105 appears grossly exaggerated in the linear drift map because the data density is insufficient to account for the complex shape of the ground water surface near two extraction wells.
4. In areas of low data control, near single or multiple stresses, the linear and linear-log drift particle tracks differ markedly. In particular, near 03EW2102 and 03EW2106, the linear drift map shows no drawdown, and consequently, no particles are

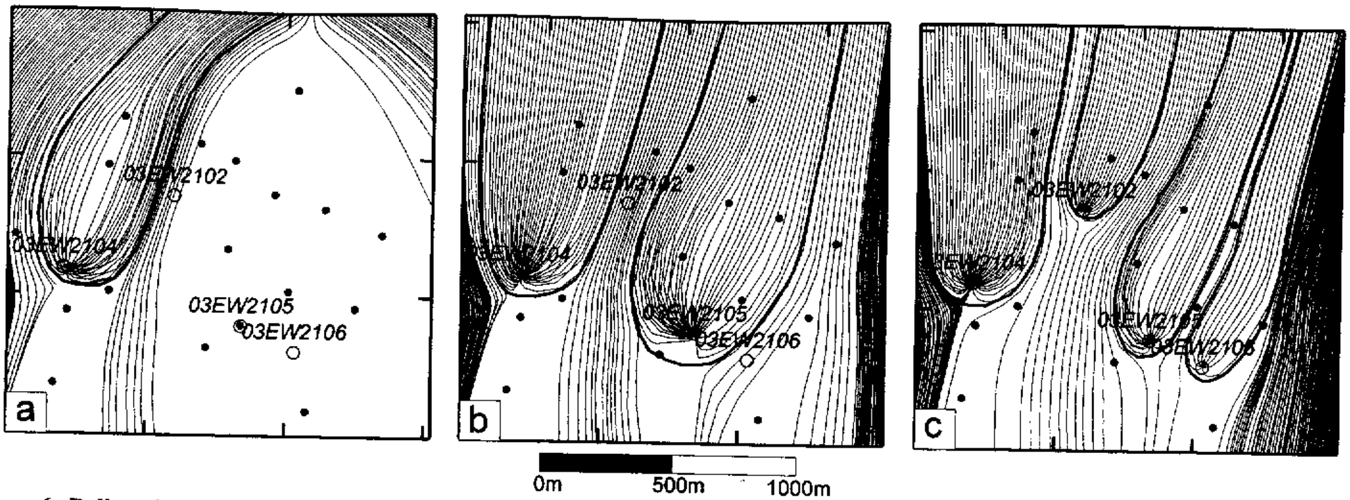

Figure 6. Delineation of well-capture zones by particle-tracking analyses: (a) no-drift, (b) linear-drift, and (c) linear-log drift.

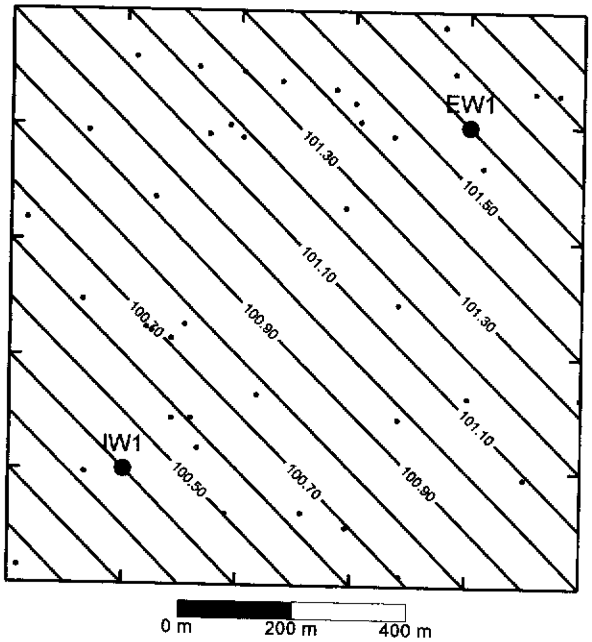

Figure 7. Example of well arrangement and uniform regional gradient.

removed at these sinks. This situation contradicts operations and maintenance information indicating that these wells were operating at their design extraction rates.

In this example, the linear-log drift generated a gridded dataset that is more representative of the physical conditions expected in the modeled domain and suitable for particle-tracking analysis for preliminary estimates of well-capture zones. This improvement arises largely from the closer approximation of conserved flow conditions calculated with the linear-log drift and provides a defensible basis for using the gridded surface to conduct particle-tracking analyses. Deviations from conserved flow are largely determined by the magnitude and distribution of residuals from the linear-log drift model and violations of assumptions underlying the Theis approximation.

Analysis of the effects of grid discretization on estimation of well-capture zones using the linear-log method is not entered into here. These can be expected to be comparable to those effects arising in two-dimensional finite difference ground water modeling, as described by Zheng (1994). In general, "ideal" grid dis-

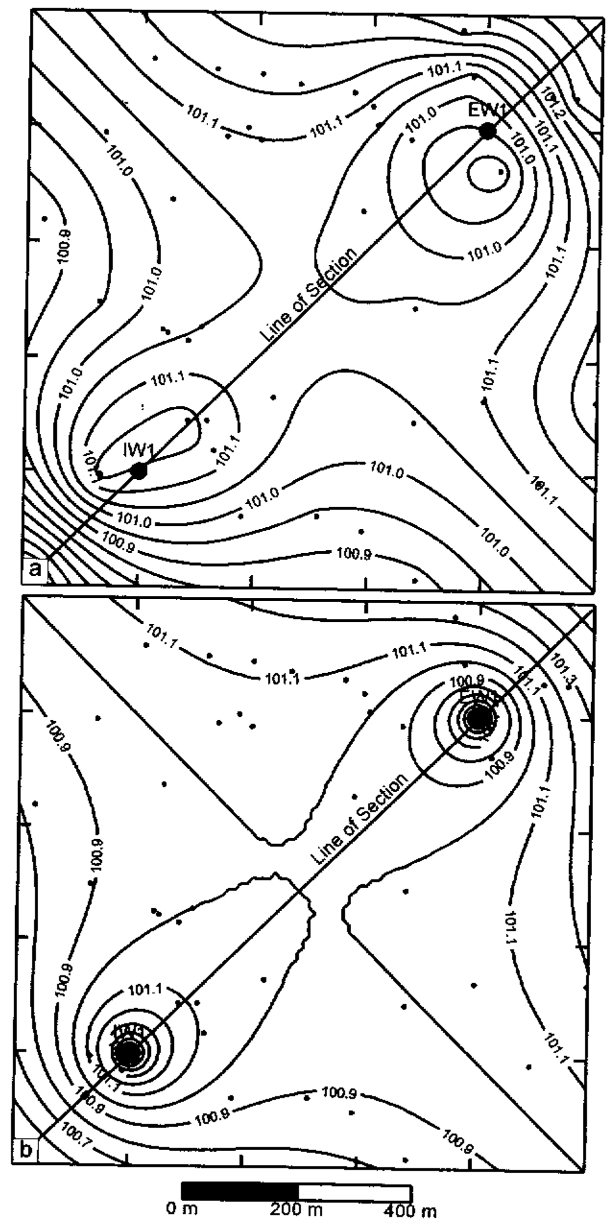

Figure 8. Ground water elevation contours calculated from linear and linear-log drift models.

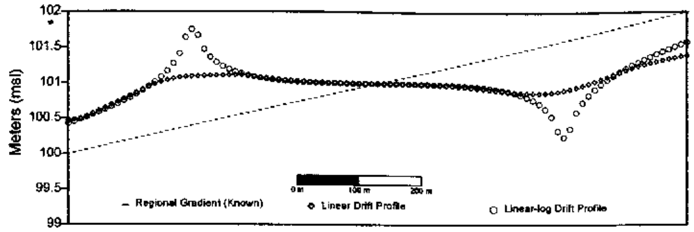

Figure 9. Profile of regional hydraulic gradients calculated from linear and linear-log drift models.

cretization is proportional to the magnitude of the source(s) and sink(s) simulated and, in this respect, is case specific.

Regional Hydraulic Gradient

Accurate estimates of the background, or regional, gradient are particularly important where compliance objectives for pump-and-treat systems include restrictions on gradient changes outside the impacted area. A linear drift can be considered as a least-squares fit of a planar surface to the ground water levels. To reduce the overall error throughout the gridded domain, the kriging routine may calculate an unrealistic underlying trend that is biased by the location of monitoring wells near pumping wells. By way of example, Figure 7 shows an artificially generated uniform background potentiometric surface. The area of interest is 1000×1000 m. Superimposed on this surface are (1) a well extracting 3.15×10^{-2} m^3/sec in the northeast (upgradient) quadrant, and (2) a well injecting 3.15×10^{-2} m^3/sec in the southwest (downgradient) quadrant. The underlying uniform hydraulic gradient, from northeast to southwest, was generated with the equation

$$h_{ij} = 100 + 0.001X + 0.001Y \tag{8}$$

where h is the elevation at location (i, j); X is the x coordinate; and Y is the y coordinate.

The resultant ground water elevation is then

$$h_{ij} = 100 + 0.001X + 0.001Y + s_{ij} \tag{9}$$

where s_{ij} is the net drawdown/mounding at (i, j) in response to pumping.

Ground water elevations were calculated at 40 imaginary monitoring wells within the domain, the locations of which were generated from a two-variable uniform random field. Drawdown and mounding at each point was calculated using Equation 4. Ground water elevation contours were then constructed by gridding the water levels at these 40 points, using the linear and linear-log drift models. Because this imaginary dataset is constructed using the theory explicit in the linear-log drift model, the linear-log kriging routine can be expected to exactly represent the structure present. Perhaps the most notable difference is that, in the linear-drift figure, the centers of highest drawdown and mounding are removed from the extraction and injection wells, respectively (Figure 8). This effect would be overcome by measuring water levels in the extraction and injection wells. However, water levels measured in pumping wells are often unrepresentative of levels in the formation adjacent to the well screen due to well losses. This circumstance is particularly evident in injection wells that have suffered severe fouling and resultant loss of efficiency.

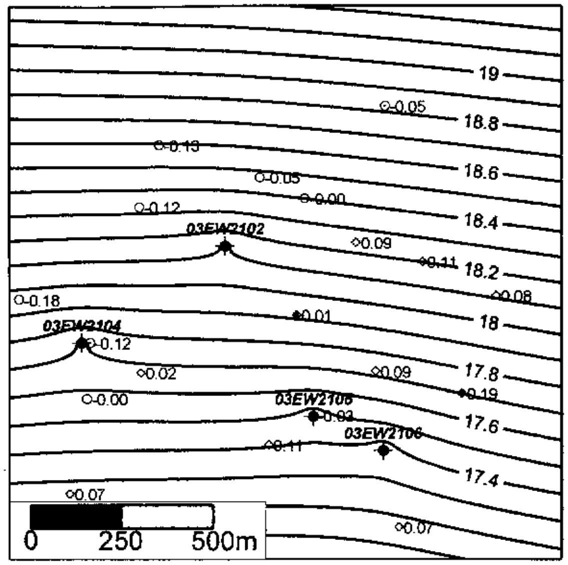

Figure 10. Contour map of linear-log drift model and posted residuals.

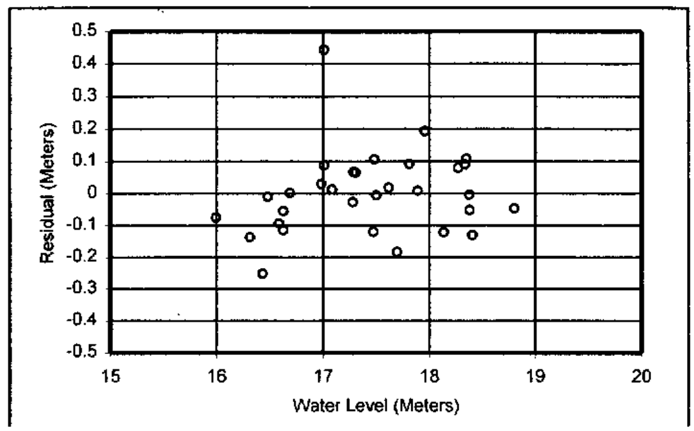

Figure 11. Residual versus water level, Cape Cod dataset.

In profile, the calculated surfaces differ markedly (Figure 9). The surface generated from the linear-drift model is perhaps best described as muted. In the area upgradient (northeast) of the extraction well and downgradient (southwest) of the injection well, the slope diverges from the known uniform background gradient. Alternatively, the surface generated from the linear-log model displays the characteristic cones of impression and depression around the injection and extraction well, respectively; at the margins of the gridded domain, the slope is converging asymptotically (logarithmically) on the uniform background gradient. Because the combined regional-linear and point-logarithmic drift specifically accounts for the drawdown and mounding, distribution of the residual error throughout the domain does not significantly affect the calculated background hydraulic gradient. The coefficients of the fitted linear drift surface (Equations 7 and 8) are 100.88 (A), 0.00045 (B), and 0.00043 (C) m, respectively—here the gradient coefficients B and C are ~50% of the known gradient coefficients.

Residual Error and Semivariogram Selection

Sources of residual error fall into two broad categories: measurement error and model error (which includes deviations of the test data from model assumptions). This paper does not include a rigorous investigation of error because the primary intention is to

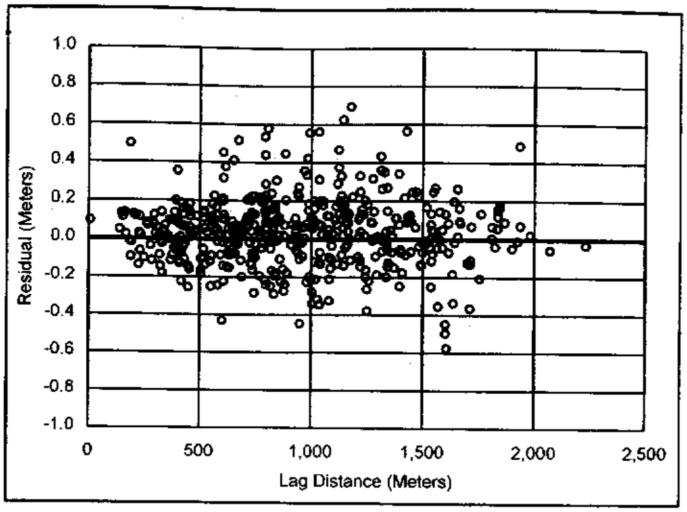

Figure 12. Residual versus lag-distance for paired monitoring points, Cape Cod dataset.

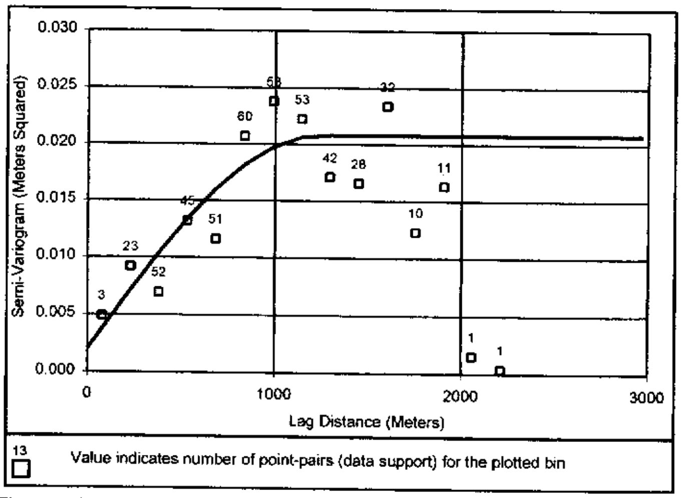

Figure 13. Calculated semivariogram of residuals from linear-log drift model.

outline some clear advantages of the linear-log approach. To accomplish this, a comparative analysis of model suitability and accuracy is provided.

As indicated previously, drift model parameters are calculated from a global estimation of Z(u). The spatial distribution of residuals is perhaps best appreciated using a horizontal (pure nugget) semivariogram, contouring the drift model and posting the residuals. This approach is possible because, although kriging is an exact interpolator at the measured data locations, point kriging at estimation locations removed from the data eliminates discontinuities at the measured data locations and provides a map of the least-squares drift model surface. This realization is presented for the linear-log model (Figure 10) but not the linear-drift model, which is simply a uniform gradient from north-northeast to south-southwest.

For the Cape Cod dataset, the residuals do not appear closely related to water level (Figure 11) or lag distance (Figure 12), nor is any residual trend or global correlation structure immediately apparent. This result is expected because estimation of the trend surface assumes the residuals to be uncorrelated. At first glance, a dilemma may appear unavoidable when selecting a suitable semivariogram model; however, residuals can be expected to show local correlation. The calculated semivariogram for the residuals from the linear-log drift is presented as Figure 13, together with an example spherical model (bin-width = 150 m). This semivariogram plot spans the entire dataset and was constructed using equi-width bins such that the number of point-pairs (i.e., weight or support) representing each plotted point varies greatly. Plotted values for separation distances greater than 1650 m are supported by fewer than 15 point-pairs; in particular, the last two are each supported by only one point-pair. Beyond this distance, the combined impact of lack of support and boundary effects render the semivariogram untenable. This supports the conclusion that the covariance is typically not well known (or estimatable) beyond one-half the field size (Deutsch and Journel 1998), and hence that the "best" results should be achieved using a semivariogram addressing only half the field size and a search-radius of one-quarter the field size. For the Cape Cod dataset, wells to the southeast may be affected by ground water extraction activities several thousand meters to the southwest that are not explicitly included in the drift model used.

For the Cape Cod dataset, the most visually appealing results are achieved using a short-range linear or spherical semivariogram to describe the near-field variance. Maps of grids created with default horizontal (i.e., the drift), linear, and spherical residual semivariograms are presented for comparison (Figure 14). The linear and spherical-model semivariogram maps are quite similar in appearance, which is probably because the spherical semivari-

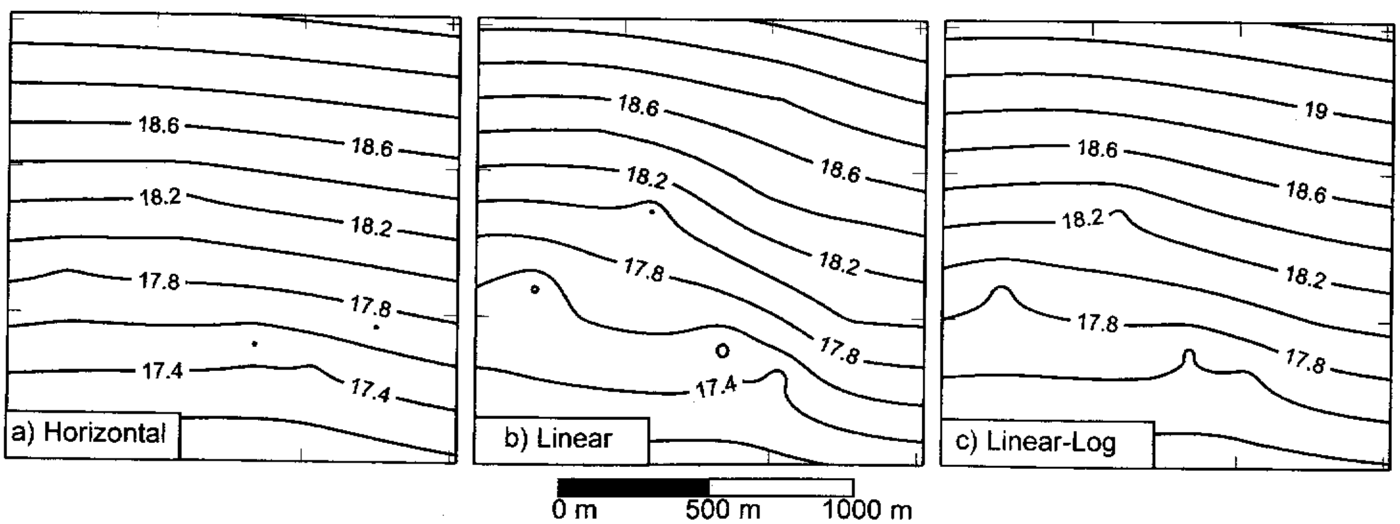

Figure 14. Water-level contours constructed with (a) horizontal, (b) linear, and (c) spherical semivariograms in addition to the linear-log drift.

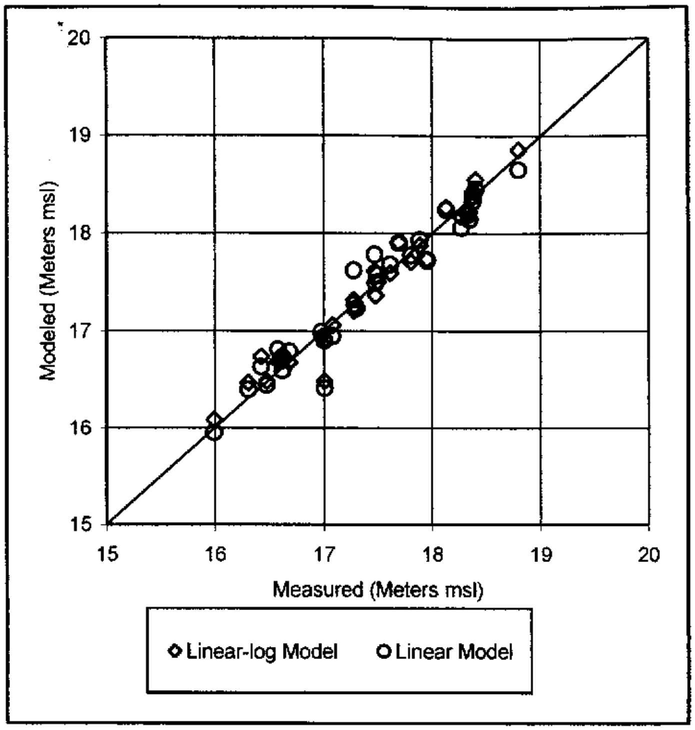

Figure 15. Measured versus modeled water level from the jackknifing analysis.

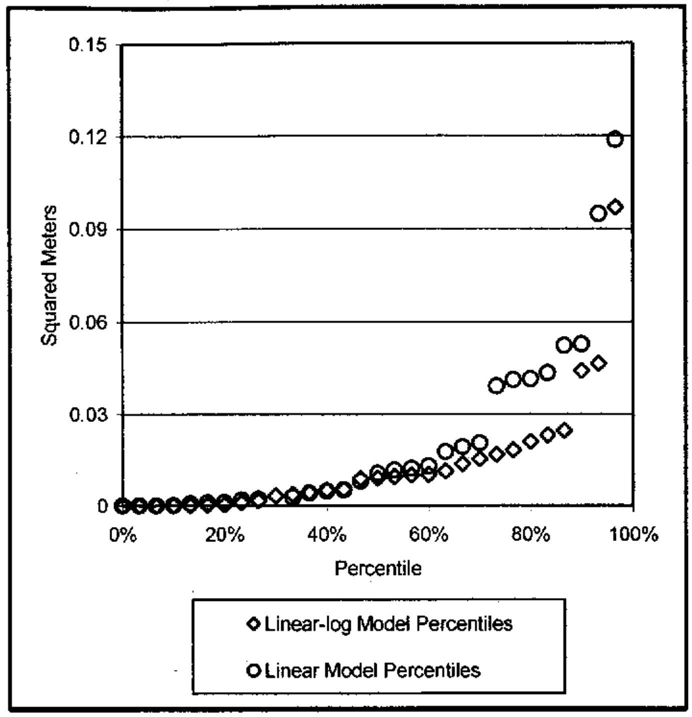

Figure 16. Percentile plot of squared residuals from the jackknifing analysis.

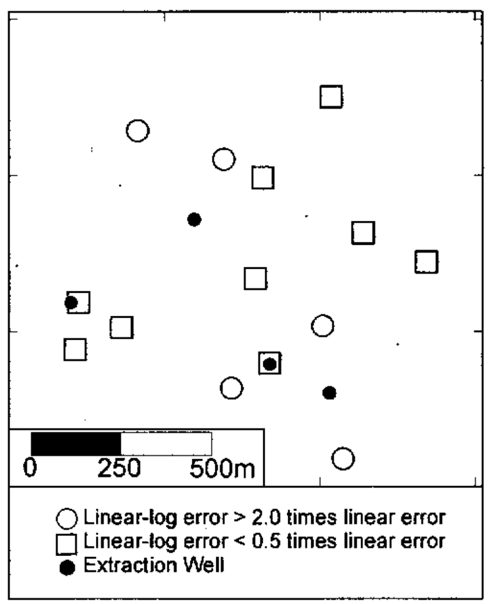

Figure 17. Map of relative error from the jackknifing analysis.

ogram is linear at low lag distances. The commonly cited log-normal approximation for the distribution of many hydrogeologic properties, such as hydraulic conductivity (Roth 1998), might suggest an exponential semivariogram is also an appropriate selection. However, experimentation with a number of different water-level datasets kriged using the linear-log drift model and various residual semivariograms suggests that, typically, linear and spherical semivariograms produce maps that describe the data satisfactorily and quickly return to the drift outside the convex data domain. For purposes of this study, the maps used for the particle-tracking exercise mentioned were created in a single kriging step using a default linear semivariogram; however, the authors suggest that appropriate semivariogram selection and fitting should be conducted as part of any rigorous study of ground water level data.

Jackknife Model Comparison

The uncertainty related to kriging approaches (or models) is often assessed by mapping the kriging standard deviations and/or the Lagrange multipliers. These are intimately related to the modeled semivariogram parameters, i.e., the sill, nugget, and range, and are not directly influenced by the form of drift model used. The form of the kriging equation (Equation 1) can be considered as two "stacked" models, i.e., the expression representing the drift term, and an expression (or series of nested expressions) representing the residual semivariogram. The linear-log drift approach represents a revision of the drift term (m[u]) and does not directly affect the methodologies for modeling of the residual (R[u]) component, which in either the linear-log or linear case is modeled as a single or series of stacked analytical approximations to the calculated semivariogram. Ideally, of course, if a "better" drift model is used, the calculated residuals may be smaller, resulting in a smaller variance and smaller kriging standard deviations. However, semivariogram modeling can be a subjective exercise, and comparison of kriging standard deviations and/or Lagrange multipliers includes this subjectivity. For this reason, the authors have attempted in the following to present a concise comparative analysis of model errors arising from the linear-log and linear drifts alone (i.e., errors related to modeling the m[u] term) and avoid a discussion of errors related to semivariogram modeling.

Numerous methods of varying complexity are available to assess or compare the correctness of model structure. Principal among these in geostatistics is jackknifing (or single-point cross-validation). In this method, each data point is, in turn, suppressed (removed from the dataset) and estimated using the kriging model based on the remaining data. The differences between the measured value and estimated values can be squared and summed, and this value used to indicate the accuracy of the model. This approach has been used to compare the linear-log and linear-drift models, by estimating the value of the drift component of Equation 1 at each suppressed point, in turn, and summing the squared differences. The calculated sum-of-squared differences are 0.67 and 0.97 m^2 for the linear-log and linear-drift models, respectively. The scattergram (Figure 15) and rank-percentile plot (Figure 16) further support the conclusion that the linear-log drift model is a better model, or predictor, of the measured water levels.

As outlined in Gaganis and Smith (2001), errors arising from the imperfect mathematical representation of the structure of a hydrologic system, i.e., model error, are not random but rather systematic. A review of model error may elucidate the form of this systematic error, or model bias. For the Cape Cod dataset, the squared residuals calculated from the jackknifing approach have been mapped in Figure 17. Where data are available adjacent to the extraction wells, the linear-log error is less than half the linear error (indicated by a square); away from the extraction wells, the pattern appears more random. This simple comparison supports the intuitive conclusion that residuals from the linear-drift model are biased high adjacent to the extraction wells, where the form of the drift model is unable to represent the shape of the depressed potentiometric surface.

Further analysis of the residuals might indicate that their magnitude and distribution reflect deviations of field conditions from the assumptions implicit in the linear-log drift model, such as aquifer homogeneity, isotropy, and well penetration. If hydraulic conductivity data are available throughout the modeled domain on a frequency equal to or greater than that of water-level data, cokriging the water levels with colocated hydraulic conductivity data (Deutsch and Journel 1998) might indicate the distribution of error is correlated to hydraulic conductivity by reducing overall error.

Parameter Estimation

Although a priori knowledge of aquifer properties such as transmissivity (T) and storage coefficient (S) is not required or explicitly included within the kriging routine presented, knowledge of these properties from long-term pumping tests provide valuable means of verifying, for example, capture zones calculated using the kriged ground water surface. By restructuring the linear-log drift with the explicit inclusion of T, it should be possible to elucidate the optimum value of T matching the measured data. This possibility suggests a potential for linear-log kriging as a parameter estimation procedure, although this has not been investigated by the authors at this time.

Conclusions

The purpose of this paper is to introduce a simple, single-step kriging routine that improves on existing methods used with two-dimensional water-level data. The linear-log kriging approach was developed as a practical solution to improving the level of interpretation possible from measured ground water level data. Providing that violations of the assumptions accompanying the Theis approximation are limited, application of the method described herein provides a gridded ground water surface suitable for tracking particles to estimate well-capture zones. The surface created comes closer to conserving flow than when a linear drift is used. Preliminary estimates of well capture can be made within moments of water-level measurement. For an ideal homogeneous, isotropic aquifer with fully penetrating wells, the gridded surface may be considered as a calibrated, two-dimensional model of the potentiometric surface. In cases where these limiting assumptions are fairly well adhered to, consideration of the effort and accuracy of numerical modeling (versus the method described) might indicate the latter to be a more cost-beneficial approach to estimating plume capture. Additional potential exists for a single-step estimation of aquifer transmissivity.

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The authors wish to thank the reviewers for their insightful comments: In particular, those of Greg McNulty prompted the jackknifing analysis that solidified the manuscript.

Further Information

Copies of the compiled FORTRAN and Visual Basic executables used in preparation of this report are available by contacting Matthew Tonkin at the address provided.

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Attachment 2

Documentation and Verification Package for TransientTracker

Documentation and Verification Package for:

TransientTracker

A Program for Conducting Particle Tracking

$\Sigma^2\Pi$

Contents

List of Figures

Outline

This document describes a program, TransientTracker, for calculating approximate travel paths. TransientTracker requires as input at least one grid of hydraulic head. This grid can be generated by any number of methods including: interpolation of observations, analytical solutions, and numerical simulation results.

Use of the program should be accompanied by review of the references and disclaimer provided at the end of this Documentation and Verification Package.

TransientTracker is programmed in Fortran 90/95 using a modular program structure. TransientTracker has been developed to be independent of any specific model platform, requiring simple ASCII input files and producing ASCII output files. The programs can be obtained free of charge, together with an example data set, by writing to matt@sspa.com. The performance of TransientTracker has been tested in a variety of applications. Future applications, however, might reveal errors that were not detected in the test simulations. Users are requested to notify matt@sspa.com of any errors found in this document or the programs.

1 TransientTracker

1.1 Background

Particle tracking has been implemented in TransientTracker to support approximate evaluations of historic and future contaminant migration; of hydraulic capture zones developed by pump-and-treat type remedies; and other analyses that benefit from the ability to track particles on a surface. Inputs required to execute particle tracking using TransientTracker are described in the following section. The particle tracking implemented in TransientTracker is currently only compatible with 2-D surfaces, which must be provided to TransientTracker as a formatted input.

Particle tracking uncertainty, associated with the physical process of hydrodynamic dispersion and mixing, is incorporated through a random walk component. The random walk movements are added to the advective displacements, providing an indication of the expected uncertainty in particle location due to dispersion. Larger numbers of particles will provide a better representation of the potential for plume spreading due to dispersion, but will add significantly to computation time.

1.2 Approach

Particle tracking is implemented using the fourth-order Runge-Kutta (RK4: *Press et al.* 1992) numerical integration (particle tracking) scheme, calculated upon hydraulic head surfaces that have been generated using any number of methods including analytical solutions, interpolation of observed values or a numerical simulation such as MODFLOW (*McDonald and Harbaugh* 1988). This particle tracking approach can be used to indicate the (relative) timing of the arrival of contaminants at potential receptors and/or points of calculation (POCs). This particle tracking approach is based upon that implemented in the MODFLOW-compatible particle-tracking code Path3D (*Zheng* 1992), which has been demonstrated to provide very similar results to the USGS particle tracking program MODPATH (*Pollock* 1994). The RK4 scheme that is being employed also incorporates Random-Walk (RW) approaches for representing the spreading of contaminants through time due to dispersive effects (*Prickett et al.* 1981; *Zheng and Bennett* 2002). Either of the approaches, *Prickett et al.* (1981) or *Zheng and Bennett* (2002), are available, selected by a flag in the input file (see input instructions below). It is noted that these methods are not mass conservative – that is, while they can consider the affects of advection, retardation and dispersion, they do not consider or conserve the mass of contaminants that are in the groundwater. The method employed by TransientTracker offers a rapid, visual means, of assessing the potential uncertainties in solute transport directions, which will be critical for efficient evaluation of large numbers of potential scenarios and assessing impacts of parameter uncertainty.

TransientTracker uses the linear-log kriging (pumping well drift) approach of *Tonkin and Larson* (2002) to calculate a more reasonable representation of the velocity field near pumping wells compared with a bilinear interpolation scheme (Figure 1. In addition, the velocity field converges on the well (Figure 2), which can be expected to produce more reasonable capture zones.

1.3 Principal Program Routines

The principal routines in the code are listed below, along with brief descriptions.

rkasc: (and rk4) These two routines perform a 4th Runge-Kutta solution to determine the future particle location. The routine rkasc monitors truncation error and performs step-size adjustment, while rk4 handles the multiple calls to the velocity-interpolation routine, accumulates the multiple estimates and weights them to provide the updated particle location.

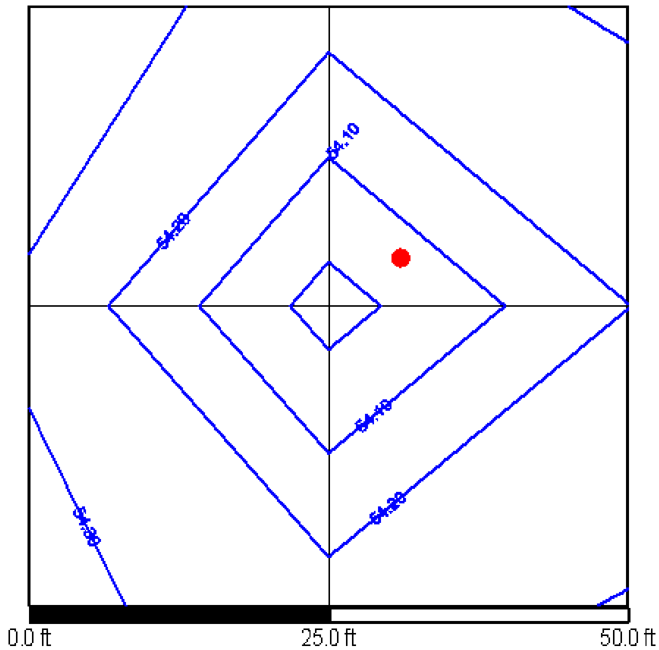
vpoint: This routine performs simple linear interpolation of velocity between gridnodes. The routine also checks for strong sinks, or strong sinks in adjacent cells. When evaluating velocity in weak-sink cells the routine invokes an analytical solution to determine the velocity vector within a cell.

krig: Kriging algorithm from *Skrivan and Karlinger* (1977) used to calculate velocities for particles near wells according to the method described by *Tonkin and Larson* (2002).

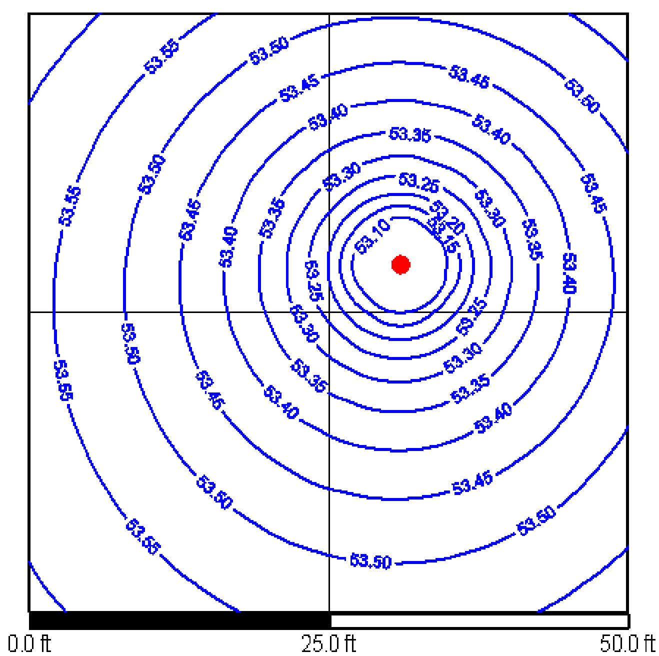
pzdispersion: Particle dispersion is implemented through this routine using either *Prickett et al.* (1981) or *Zheng and Bennett* (2002) depending on the flag setting in the input file. This routine is not invoked if all dispersivities are set to 0.0 in the input file.

1.4 Input

TransientTracker reads up to four types of input files. The first one is the main input file, TransientTracker.in, and is required and must have the default name. The other three types are Surfer grid files (GRDFILES), Well files (WELFILES), and Sink files (LINEFILES). All of these files are listed by name in TransientTracker.in.



(a) Bilinear interpolation



(b) Linear-log Kriging

Figure 1: Example head surface near a pumping well (red circle) calculated using a) bilinear interpolation and b) linear-log kriging.

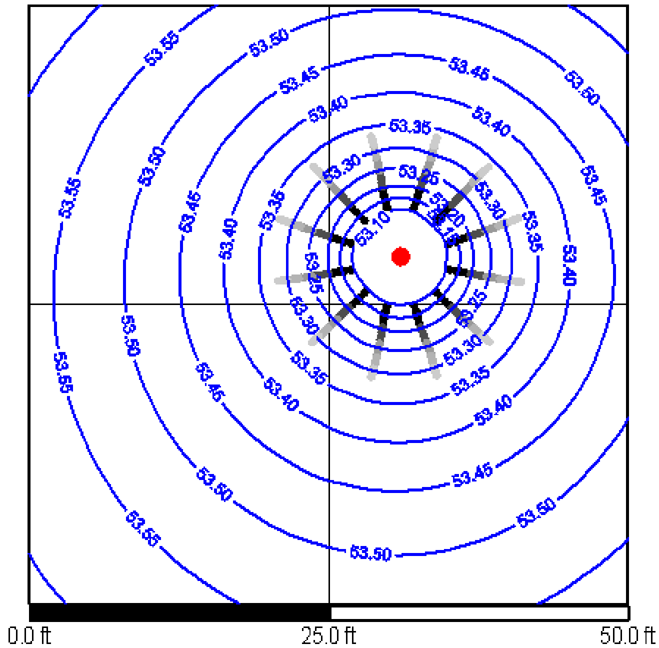


Figure 2: Example particle tracks using the linear-log kriging approach.

The following table provides a summary of the variables required in the default input file, TransientTracker.in, in the format required by the code. The indices indicate the order in which the variables are listed in the file, a new line for each successive index, with some variables requiring multiple lines of input. Text in lowercase-bold are character variables: they need to be entered exactly as provided in the table, followed by the variables indicated. The input is free format: entries do not need a specific spacing on each line, and multiple entries on a line should be separated by one or more spaces.

Index	Variables
1	**ngrd** NGRD
2	**ncol** NCOL
3	**nrow** NROW
4	**xmn** XMN
5	**ymn** YMN
6	**zmn** ZMN
7	GRDFILES(i), WELFILES(i), LINEFILES(i), TTIME(i): This line is repeated NGRD times
8	IBACK, NPTP, COND, POR, STEP, NPART, XPRAD, NRADS, NOUT, MAXTIME
9	ALPL, ALPT, PORZ

10	ROERR, TINY, SAFETY, EPS, VSMALL, COURANT, SINK STRENGTH
	Items 11 or 12 are entered depending on the value of the NPART flag
11a	**nparticles** NPARTICLES
11b	XPSTART(j), YPSTART(j): This line is repeated NPARTICLES times.
12a	**space** SPACE
12b	**xmn** XMIN
12c	**xmx** XMAX
12d	**ymn** YMIN
12e	**ymx** YMAX

The following provides an explanation of the variables required in "Transient-Tracker.in" and some of the options regarding the possible values.

Variable	Description
NGRD	Specifies the number of grid files to be used by the program. Typically one grid will reflect a steady-state flow field and multiple grids reflect changing flow conditions with changing stresses.
NCOL	Number of columns in the Surfer grid files
NROW	Number of rows in the Surfer grid files
XMN	Minimum value of the x-coordinate nodes: the x coordinate of the node in the 1st row, 1st column
YMN	Minimum value of the y-coordinate nodes: the y coordinate of the node in the 1st row, 1st column.
ZMN	Minimum value of the z-coordinate
GRDFILES	Name of each Surfer grid file
WELFILES	Well file names
LINEFILE	Names of each line-source file
TTIME	Termination time, time at which the associated grid file ceases to apply
IBACK	Flag for selecting forward or backward tracking. 1 for forward tracking, -1 for backward tracking
NPTP	Total number of particles transport steps to simulate
COND	Hydraulic conductivity of the porous medium [L/T]. NOTE: this value must be in units that are consistent with the flow simulations that generated the piezometric surface that was gridded using Surfer
POR	Porosity of the porous medium

STEP	Transport step size for moving particles
NPART	
XPRAD	Placeholder value for future use
NOUT	Transport step interval for output, e.g., NOUT = 5 will produce output every 5th transport step
MAXTIME	Maximum simulation time
ALPL	Longitudinal dispersivity [L]. NOTE: this value must be in units that are consistent with the flow simulations that generated the piezometric surface that was gridded using Surfer
ALPT	Transverse dispersivity [L]. NOTE: this value must be in units that are consistent with the flow simulations that generated the piezometric surface that was gridded using Surfer
PORZ	Flag to indicate which formulation of the random-walk dispersion approximation is used: PORZ = 0 for *Prickett et al.* (1981), or PORZ = 1 for *Zheng and Bennett* (2002)
ROERR	Round-off error cutoff for Runge-Kutta integration (recommended = 1.0 E-04)
TINY	Stagnation and minimum tracking time criterion for Runge-Kutta integration (recommended = 1.0 E-10)
SAFETY	Stepsize adjustment criterion for Runge-Kutta integration (recommended = 0.80)
EPS	Error criterion scaling factor for Runge-Kutta integration (recommended = 1.0 E-06)
VSMALL	Placeholder value for future use. (recommended = SQRT(EPS))
COURANT	Particle step control. If the updated particle location moves a particle more than 1 cell length, the step size is recalculated using the courant number according to: $\frac{courant \times cell\ size}{magnitude\ of\ velocity}$
SINKSTRENGTH	Used to flag low-points in the flow field that are not the result of a well or line-sink. These low-points are stagnation areas for particles and cause lengthy runtimes if a particle is allowed to “bounce” around in these areas. The strength is a head difference. That is, if the head at a node is more than SINKSTRENGTH less than the value of the four surrounding nodes, that node is flagged as an internal sink
NPARTICLES	Number of particles to simulate if NPART is 1
XPSTART	Starting x-coordinate location for particle
YPSTART	Starting y-coordinate location for particle
SPACE	If NPART is 0 then a regular grid of particles is simulated. SPACE is the spacing between particles for this grid
XMIN	minimum x-coordinate for particle location grid
XMAX	maximum x-coordinate for particle location grid
YMIN	minimum y-coordinate for particle location grid

YMAX	maximum y-coordinate for particle location grid

GRDFILES(i) The Surfer input files, the GRDFILES(i), listed in TransientTracker.in, are grids of the groundwater levels from each timestep of the numerical simulation. The grids are associated with the total elapsed simulation time (TTIME(i)) at the end of each respective timestep. To avoid potential issues with location referencing, all grids must have the same dimensions and origins. Formatting instructions for creating Surfer ASCII files is includedin Appendix A of this manual.

WELFILES(i): The files defining the locations and characteristics of each well are simple ASCII files and provide information in the following format:

Index	Variable
1	NWELLS
2	qxx(i),qyy(i),qqq(i),qrad(i),idtwell(i),qtype(i),wellname(i) where this line is repeated NWELLS times.

The parameters listed above have the following definitions:

Variable	Description
NWELLS	Specifies the number of wells files that are active during this timestep: the wells that influenced the current grid file.
qxx(i)	X –coordinate of well i
qyy(i)	Y –coordinate of well i
qqq(i)	Pumping rate of well i for the current timestep
qrad(i)	Well bore radius. Used to capture the particles as they approach the well. In some instances, especially with wells creating a very sharp cone of depression, increasing this number beyond the actual well-bore radius may help with stability of the final particle transport steps.
idtwell(i)	A well-id label
qtype(i)	Specify the well as recovery (R) or not recovery (NR)
wellname(i)	A name for the well

LINEFILES(i): These files define the locations and characteristics of sink line segments. They are simple ASCII files and provide information in the following format:

Index	Variable
1	NLIN
2	lxs(i),lys(i),lind(i),lval(i) where this line is repeated NLIN times.
3	lxe(i),lye(i),idum,rdum
NOTE: Items 2 and 3 are repeated NLIN times. If NLIN <0 then only 2 is repeated NLIN times.	

The parameters listed above have the following definitions:

Variable	Description
NLIN	Number of line segments to be read in the file. Must be less than 100, which is hardwired into the code as MAXNLIN
lxs(i)	X location of starting point(s) i
lys(i)	Y location of starting point(s) i
lind(i)	Indicator of line sink/source/'feature' type. 1 - 'river' with a const head value, 2 - 'horiz well' with const Q-in/Q-out
Lval(i)	'value' for the line feature. Head (when lind = 1), river (when lind = 1)
lxe(i)	X location of ending point(s)
lye(i)	Y location of ending point(s)
idum(i)	Check value, needs to match lval
rdum(i)	Check value, needs to match lind

1.5 Output

TransientTracker produces two output files: the particle tracks, ptrack.out, and the capture locations of each particle, capture.out. Both ptrack.out and capture.out are formatted ASCII files that can easily be imported by a plotting package such as Surfer.

The file ptrack.out provides a listing of the particle locations (x, y, time, particle number) with each transport step (or multiple of transport steps depending on the value of NOUT). A sample of the first few lines of a typical ptrack.out file is provided below:

```
0.374760000000E+04 0.413894000000E+04 0.000000000000E+00 1
0.374879680903E+04 0.413927856838E+04 0.200000000000E+00 1
0.374733118239E+04 0.413823623645E+04 0.100000000000E+01 1
```

TransientTracker includes functionality for removing particles at the margins of the grid domain; at stagnation zones; at sinks when forward tracking. The program records the fate of particles in an ASCII summary file called capture.out. The contents of this file can be manipulated to illustrate capture zones. The program uses an integer variable (IREM) to indicate if, and where, a particle was removed from the particle tracking for any of the reasons listed above. The value of this variable, as written to capture.out can be used to produce maps that illustrate the fate of the particles. Current capabilities include the removal of particles that exit the domain:

- Not captured (IREM=0)
- At the bounds of the grid (IREM=1)
- At a 2D Recovery Well (IREM=2) (QTYPE='R')
- At a 2D line sink/sources (IREM=3)
- At a stagnation point (IREM=5 or 6)
- Beyond the maximum transport-simulation time (IREM=8)
- Number of tracking steps exceeded (IREM=9)
- Internal stagnation point (IREM=10)

Non-recovery wells are typically injection wells, but may also be wells that are not pumping in a particular stress period, but were simply left in the input file for consistency. The file capture.out provides, for each particle, the starting location, exit time, exit coordinates, exit row, column and layer, and the mechanism of exit. An example of a portion of a capture.out file is provided below:

```
1 6161.9587 1761.6945 0.0000 14852.2305 3556.8680 947.477
2 5948.3987 1685.1856 0.0000 13742.2650 3557.3389 944.395
3 5626.3664 1414.9735 0.0000 11981.5765 3553.3730 953.438
4 5870.5205 1624.0371 0.0000 13106.5835 3550.3535 943.901
```

2 Program Verification Data Set

TransientTracker was verified using two analytical solutions and a set of numerical solutions of a two-dimensional transient system.

2.1 Verification with Travel Time Derived From Thiem Equation

The explicit solution of the Thiem equation for particle travel time to a well (*Neville* 2007) was used to estimate particle travel time from a variety of distances to a fully-penetrating well in a confined, homogeneous system. Results were also generated using MODFLOW and MODPATH. A Surfer grid file was made from the MODFLOW-calculated potentiometric surface. Particle tracking using TransientTracker and the Surfer grid file was performed to create a third set of results. All three sets of results are included in Figure 3.

The results shown in Figure 3 demonstrate excellent agreement between the three methods. The parameters used for this simulation are listed in the table below.

Parameter	Value
Hydraulic Conductivity (m/day)	0.864
Aquifer Thickness (m)	10.0
Well radius (m)	0.1
Maximum travel distance (m)	100.0
Pumping rate (m3/day)	54.5
Porosity	0.35
MODFLOW Square grid-cell size (m)	2.0
MODFLOW Grid dimensions	1001 x 1001

2.2 Verification with Analytical Solution, BRICK

TransientTracker, particularly the dispersion process component, was verified by comparing the results with an analytical solution of a simple transport scenario. The analytical code BRICK (*Neville* 2006) was used to generate contours of concentration at 1000 days after an initial released from a square source zone measuring 5 feet on each side. The following inputs were specified for BRICK:

Porosity [-]	0.30
Velocity [L/T]	0.25
Longitudinal Dispersivity [L]	10.0
Lateral Transverse Dipsersivity [L]	0.1
Source zone Xmin, Xmax	-5.0, 5.0
Source zone Ymin, Ymax	-5.0, 5.0
Initial Slug Mass	1.00 E+05
Domain Xmin, Xmax, dx	-50.0, 500.0, 1.0
Domain Ymin, Ymax, dy	-100.0, 100.0, 1.0

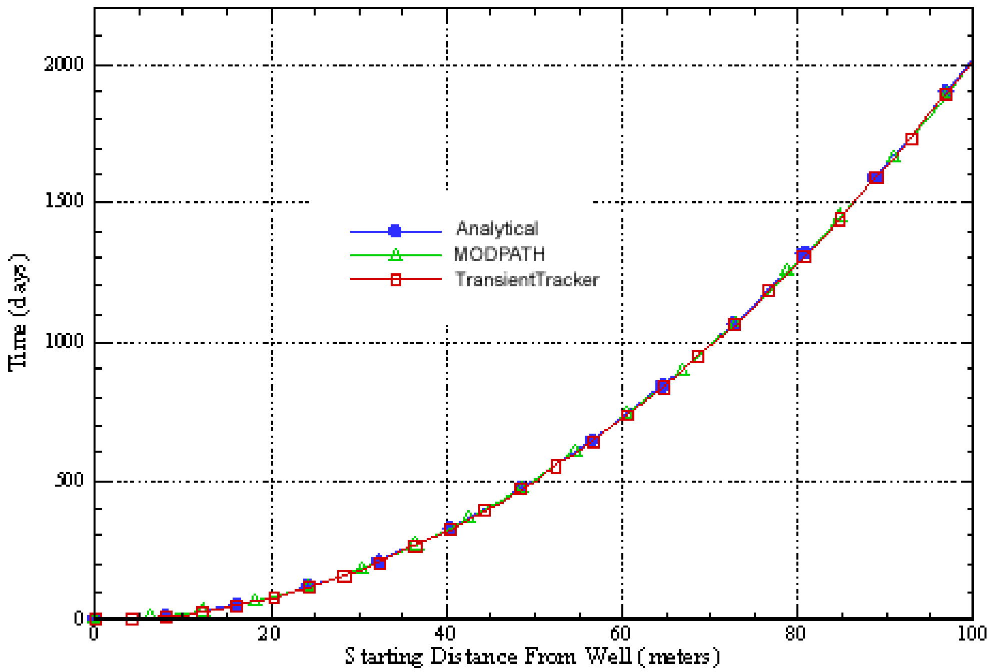


Figure 3: Travel time to reach pumping well calculated using (1) analytical solution, (2) MODPATH, and (3) TransientTracker.

Using an assumed value of hydraulic conductivity equal to 100.0, a Surfer grid file was created with the same domain extent and grid resolution as the BRICK solution. The piezometric surface generated using a gradient of 7.5 E-04, with the high values of piezometric surface along the left hand boundary (X = -50.0).

TransientTracker was run with the resulting Surfer Grid file using 1681 particles (a square of 41 x 41 particles) and dispersivity values matching the BRICK values. The file TransientTracker.in is provided below.

```
# Input file for TransientTracker benchtesting against BRICK
ngrd 1
ncol 551
nrow 201
xmn -50.00
ymn -100.00
zmn 0.
# Grid File information using 1 line for each "stress period"
fabgrid551x201.grd nowells.dat nosinks.dat 1000.
# Tracking information
1 100000 100.0 0.3 10.0 1 50.  1 1 30000.
10.0 0.1 0
1.e-3 1.e-6 0.8 1.e-6 1.0e-3 1.0 0.
# Particle Locations 1681
```

```
nparticles 1681
-5.00 -5.00
-4.75 -5.00
-4.50 -5.00
-4.25 -5.00
.........  (input continues until particle #1681)
```

The results, depicted in Figure 4, demonstrate the ability of the particle tracking routine to move the particles in accordance with the flow field, and for the random-walk to add a component of uncertainty in the simulated position of each particle. As an additional test of TransientTracker, two additional simulations were performed using the same flow field. For the first additional run, Run #2, longitudinal dispersivity decreased by a factor of 10, and for Run #3, dispersion was not simulated (Figure 5). The results are consistent with expectations. Run #2 has a decreased longitudinal spread with the same transverse spreading, and the third run is a simple translocation of the source in the uniform flow field according to advection alone.

2.3 Verification Using Numerical Solutions

TransientTracker particle tracking results were also compared to MODPATH v4.3 (*Pollock* 1994) and PATH3D (*Zheng* 1992). A rectangular, uniform-grid, two-dimensional simulation was constructed. Grid cells were 100 feet on each side. The grid had 50 rows and 100 columns. Boundary conditions consisted of three sections of general head boundaries around a portion of the perimeter, and a well that switched from injection, off, to low pumping, and then high pumping matching the initial injection rate, over the course of four stress periods (Figure 6). The first stress period was steady state, followed by 100 days of no pumping, 1000 days of low pumping and then 30000 days of high pumping. Other model-run parameters are summarized in the table below.

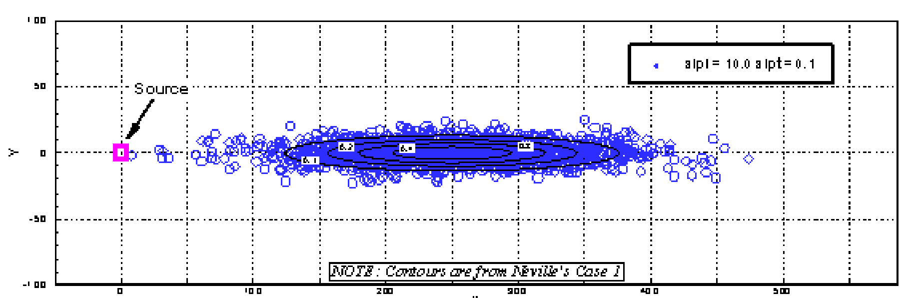


Figure 4: Particles from TransientTracker and contours from BRICK at T = 1000days.

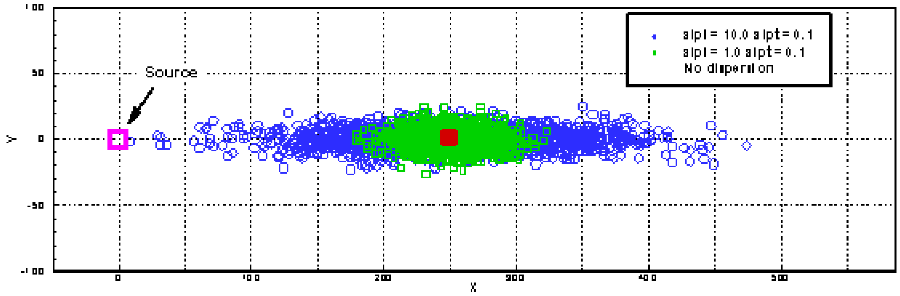


Figure 5: Particles from TransientTracker for 2 dispersivity values and zero dispersivity at T=1000days.

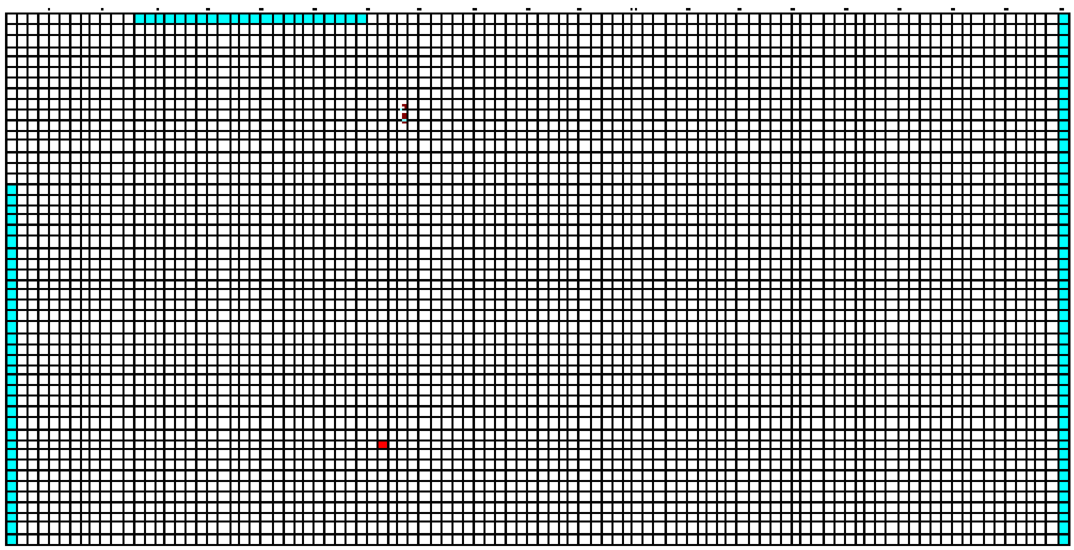


Figure 6: Test case model grid with GHB cells (blue) and pumping cell (red). Each grid cell is 100 feet on each side. The grid has 100 columns and 50 rows.

Parameter	Value
Porosity [-]	0.10
Longitudinal Dispersivity [ft]	2.5 or 0.0
Lateral Transverse Dipsersivity [ft]	0.5 or 0.0
Hydraulic Conductivity [ft/day]	100.0
Stress-period Pumping [1000 ft3/day]	50, 0, -2, -50

The following sets of figures depict results from the groundwater simulation and the particle tracking. It is worth noting that this test case is not intended to be strictly realistic: it was constructed to provide a set of groundwater surface elevations with dramatic changes in the velocity vectors over time.

Figure 7 depicts the initial steady-state groundwater surface due to the general head boundaries and the well injecting at ~250 gpm. The particle release locations are also indicated. Figure 8 shows the groundwater surface for the final stress period. Particles were released in the initial, steady-state stress period, which had a duration of 2000 days. The second stress period, without any pumping, lasted 100 days and the third, lasting 1000 days, had a pumping rate of ∼20 gpm. The fourth and final stress period pumped at a rate of ∼250 gpm and had a 30,000-day duration, allowing plenty of time for any particles to complete their travel.

A portion of the TransientTracker input file, TransientTracker.in, used in the verification runs is reproduced below. Only the first five particles are listed, and some parameters, such as dispersivity, were modified between runs.

```
# Input file
ngrd 13
ncol 100
nrow 50
xmn 50
ymn 50
zmn 0.
# Grid File information using 1 line for each "stress period"
vista3_T02000_0.grd nowells.dat nosinks.dat 2000.0
vista3_T02018_6.grd nowells.dat nosinks.dat 2018.6
vista3_T02041_0.grd nowells.dat nosinks.dat 2041.0
vista3_T02067_8.grd nowells.dat nosinks.dat 2067.8
vista3_T02100_0.grd nowells.dat nosinks.dat 2100.0
vista3_T02286_3.grd nowells.dat nosinks.dat 2286.3
vista3_T02509_8.grd nowells.dat nosinks.dat 2509.8
vista3_T02778_1.grd nowells.dat nosinks.dat 2778.1
vista3_T03100_0.grd nowells.dat nosinks.dat 3100.0
vista3_T08688_7.grd wells.dat nosinks.dat 8688.7
vista3_T15395_1.grd wells.dat nosinks.dat 15395.1
vista3_T23442_8.grd wells.dat nosinks.dat 22442.8
vista3_T33100_0.grd wells.dat nosinks.dat 33100.1
# Tracking information
1 900000 100.  0.100 0.20 50.  1 1 33100.1
2.5 0.5 0
1.e-3 1.e-6 0.8 1.e-6 1.0e-31.0 0.
# Particle Locations 100
nparticles 100
3.74760E+03 4.13894E+03 P0001
3.74772E+03 4.13733E+03 P0002
3.74785E+03 4.13572E+03 P0003
3.74797E+03 4.13411E+03 P0004
3.74809E+03 4.13250E+03 P0005
```

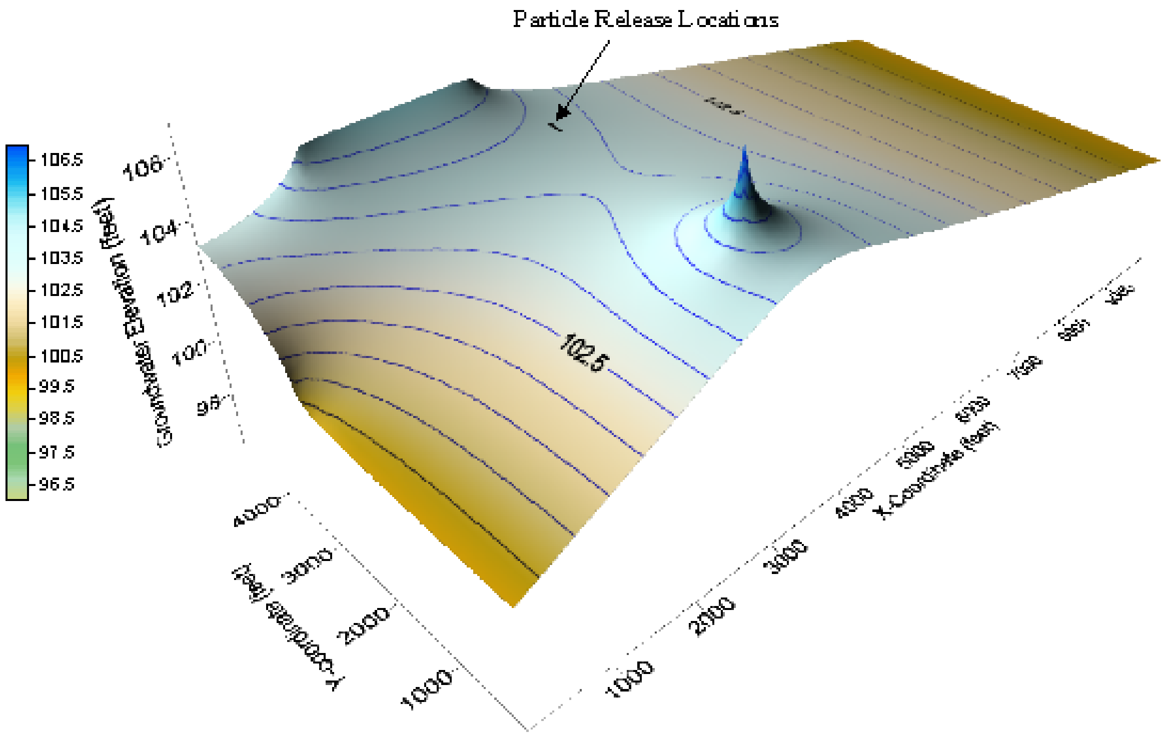


Figure 7: Initial groundwater surface.

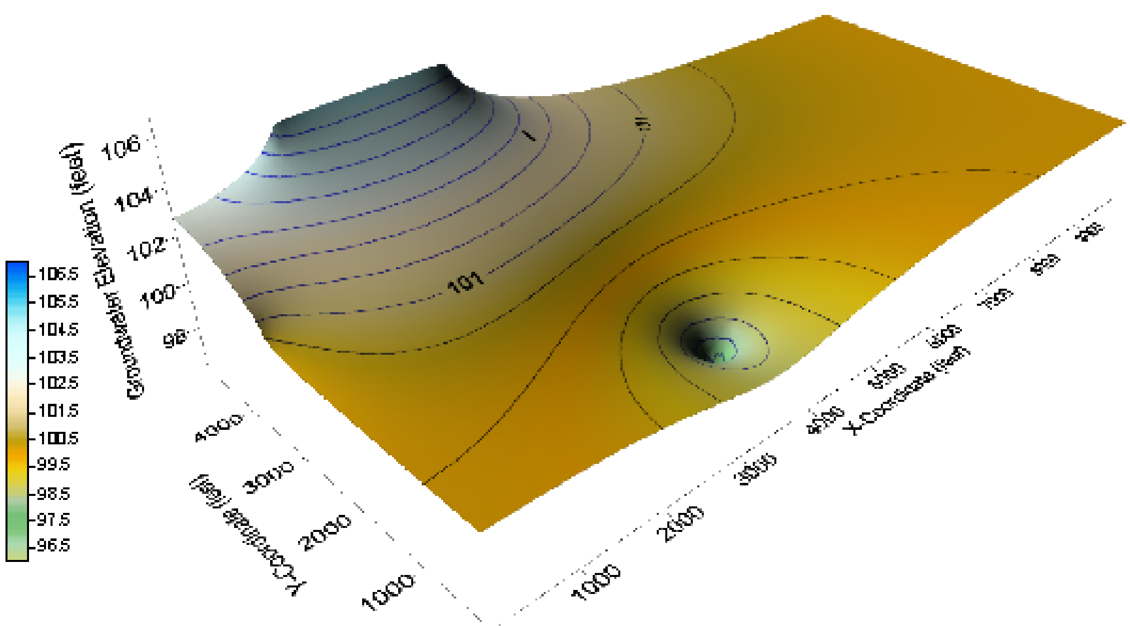


Figure 8: Final groundwater surface.

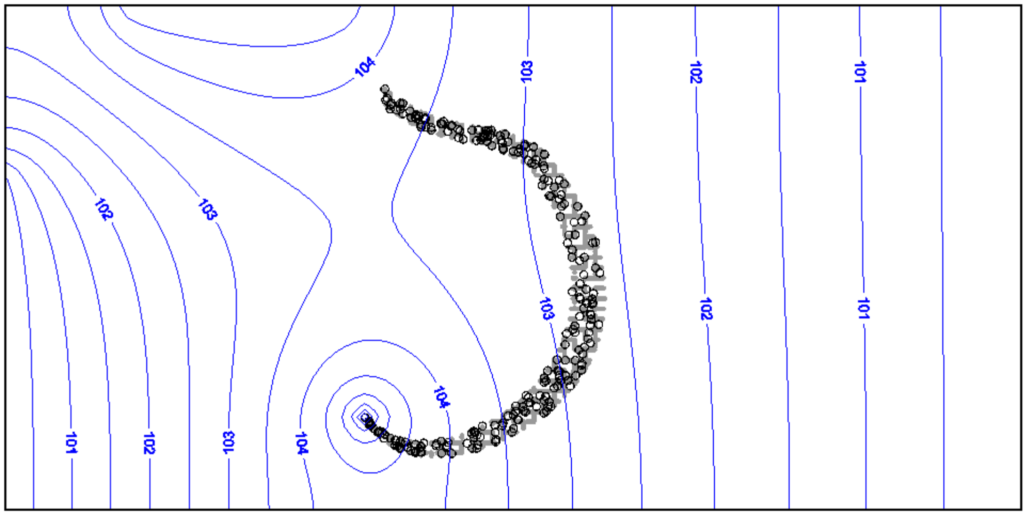


Figure 9: Comparison of TransientTracker and MODPATH results, no dispersion.

The gray particles in Figure 9 are the MODPATH particle-tracking results. The black particles are the TransientTracker results. The two methods provide nearly identical paths. Path3D results are not shown since they were indistinguishable from these results. This figure provides a demonstration that TransientTracker is capable of representing advective particle transport in homogeneous aquifers.

Particle tracks in Figure 10 demonstrate the longitudinal (2.5 feet) and transverse (0.5 feet) dispersivity impacts using the same line source and conditions as in Figure 9. Dispersion in this figure is simulated using the *Prickett et al.* (1981) random walk algorithm. In Figure 11 the same particle tracks are shown in the background, and in the foreground are particle locations at 8688.7 days after the start of the simulation. This cloud of particles illustrates the considerable differences in travel time experienced by the various particles as a result of small differences in starting location, and the simulated dispersion.

By starting all 100 particles at a single point, Figure 12 provides a comparison to Figure 11 and demonstrates that the simulated dispersion, as opposed to initial particle location, is the dominant source of spreading as the particles progress towards the well. The advection-only particle track originating from the single-point source is provided in the background (gray) for reference.

For remediation purposes, it is often helpful to assess the capture region for a given scenario. The capture.out file was used to identify locations where particles released at the beginning of the simulation would get captured by the well. The red dots in Figure 13 indicate the locations that will be captured by the well, while the blue crosses indicate locations where particles move out of the domain instead of being

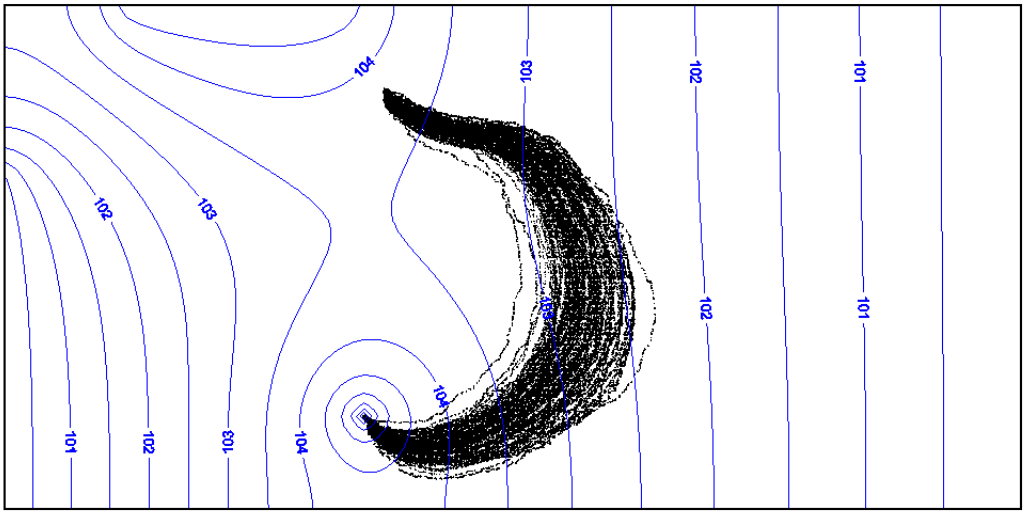


Figure 10: TransientTracker particle paths with longitudinal (2.5 feet) and transverse (0.5 feet) dispersion.

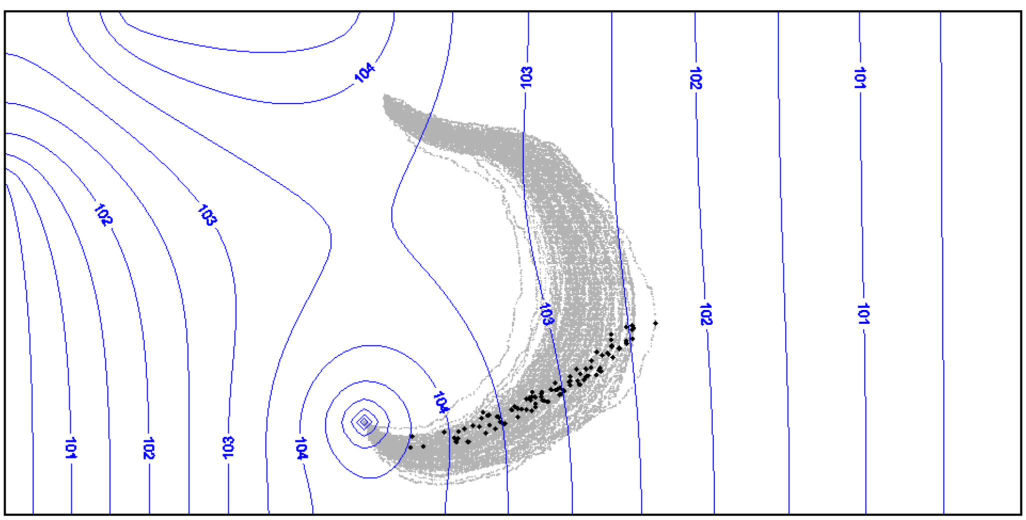


Figure 11: Particle locations (black) at 8688.7 days.

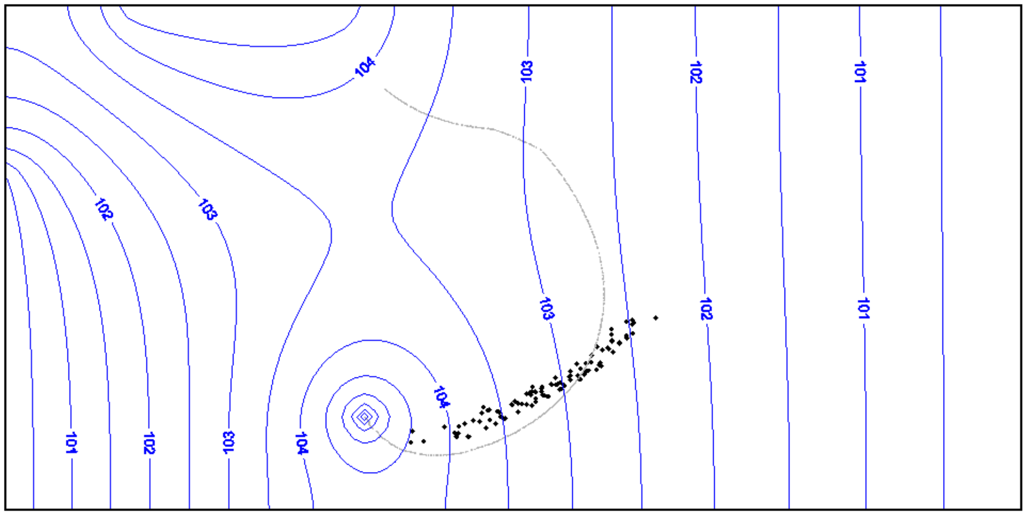


Figure 12: Dispersion impacted TransientTracker particles from a point source at 8688.7 days, with the advection-only track in the packground.

captured. While Figure 13 demonstrates the captured locations within the domain, it is important to keep in mind that this pumping well has a significant impact on the domain boundaries. This serves as an important example of how domain boundaries can affect the capture zone: additional locations from within the existing domain would be captured if the domain were extended to the point that pumping impacts were not significant at the boundaries.

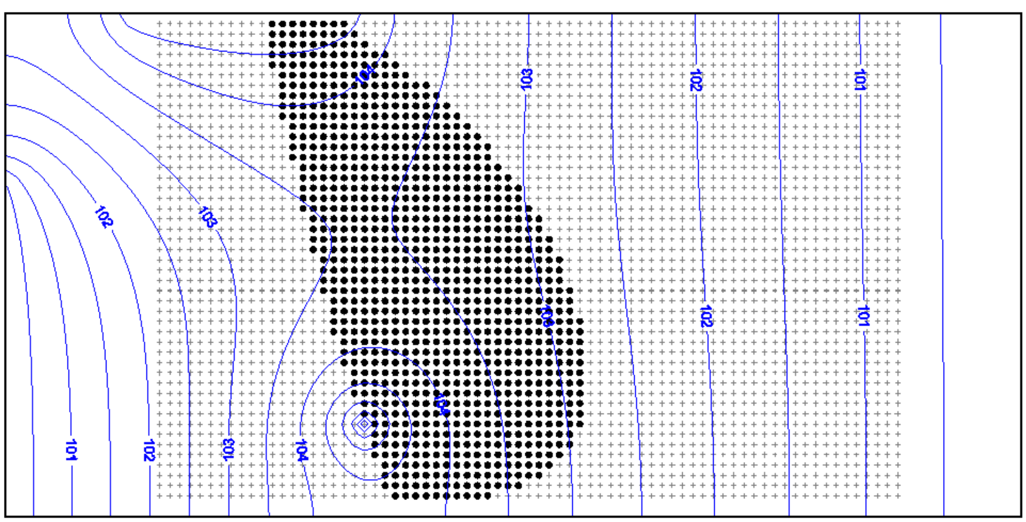


Figure 13: Capture zone indicating the locations (black circles) from which a particle released will be captured by the recovery well. Gray crosses indicate particles that leave through a domain boundary.

Technical Support

Limited technical support can be obtained by writing to matt@sspa.com.

Disclaimer

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A Surfer ASCII Grid File Format

The entries in the header and the data can be space, comma or tab delimited.

DSAA header - 'D' must be first character on first line

ncol,nrow number of columns, number of rows

xmin,xmax minimum x-coordinate of grid, maximum x-coordinate of grid

ymin,ymax minimum y-coordinate of grid, maximum y-coordinate of grid

zmin,zmax minimum data value, maximum data value

data for every node, the surface (data) value, listed in the order presented in Figure 14. Data is written in order from lower-left to upper-right (row 1, col 1 to row NROW, col NCOL). If there are 10 rows and 10 columns, 100 data values must be listed

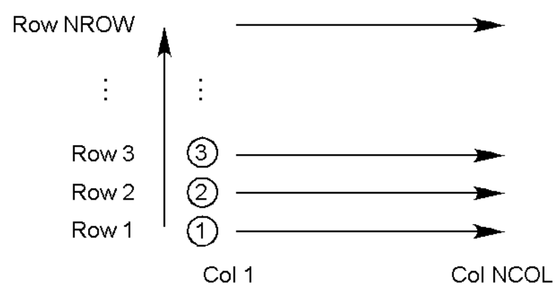

Figure 14: Order data must be written for Surfer grid file.