

Groundwater Data Utilities

Part A: Overview

Watermark Numerical Computing

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See the preface to Part B of this manual for a list of the Groundwater Data Utilities, together with a brief description of the role of each.

1. Introduction

1.1 General

In spite of the availability of powerful, user-friendly, model-specific pre- and postprocessing software, groundwater modelling is difficult. One of the main reasons for this is the necessity to transfer large amounts of data into and out of models, and between models, databases and visualisation and display software. Many an attempt to model an important groundwater system has died a “death by a thousand cuts” as the difficulties of model-related data compilation and processing tap the time, patience and resources of the groundwater modeller.

The software documented in this manual, written to complement existing models and their graphical pre- and postprocessors, was developed in an attempt to overcome some of the ancillary problems attached to the practice of groundwater modelling. None of the tasks performed by any of the programs documented herein is particularly difficult; yet to undertake these tasks without software assistance would be time-consuming and error-prone as they generally involve the processing of large amounts of data.

It is hoped that the Groundwater Data Utilities documented in this report will free modellers of some of the more laborious data-handling tasks which accompany all modelling projects, so that they may then be free to turn greater attention to the critically important issues of correct model setup, parameterisation and calibration. If this does, indeed, occur then the programming and documentation of the Groundwater Data Utilities described in this manual will have been worth the considerable effort required for their development.

1.2 The Software Environment

Many of the utilities documented in this report have been written specifically for use with MODFLOW (MacDonald and Harbaugh, 1988; Harbaugh and MacDonald, 1996; Harbaugh et al., 2000; Hill et al., 2000) and MT3D (Zheng, 1992; Zheng and Wang, 1998). With little or no modification these utilities could also be used with other cell-centred finite-difference models such as SHARP (Hedeff, 1990). Others of the utilities are model-independent, being used simply for groundwater data manipulation and presentation, whether such processing is required as part of a model-construction exercise or not.

The Groundwater Data Utilities can be used in conjunction with any MODFLOW or MT3D preprocessor. However it is an important part of the philosophical underpinning of some of the utilities that the preprocessor allow the importing and exporting of MODFLOW/MT3D-compatible, two-dimensional data arrays. Where any of the utilities documented herein read or write real or integer arrays, two slightly different conventions for formatted array storage are adopted. The first convention requires that a header line recording the number of model columns and rows precedes

the array itself in its formatted file; the second convention requires that this header line be omitted. The ability to use either of these conventions ensures that the programs of the Groundwater Data Utilities can be used in conjunction with any commercial MODFLOW GUI. The user selects the convention that he/she wishes to use in his/her work through an appropriate entry in a “settings file” - see Section 1.5 for details.

Where required by any of the utilities, grid geographical information is supplied through a “grid specification file”. This file can be easily prepared by the user based on information available through any MODFLOW GUI, and from the MODFLOW input files produced by that GUI.

Some of the Groundwater Data Utilities allow model-generated data to be interpolated and/or reformatted for importation into graphing and contouring software. Some of these utilities are independent of the user’s choice of graphing or contouring software; others, however, relate specifically to Golden Software’s SURFER package. Some of the latter utilities provide a mechanism whereby SURFER can be used in a model preprocessing role, while others enhance its ability to display model results with or without diagrammatical representation of the finite difference grid (including any zonation defined within this grid).

Functionality is included within the Groundwater Data Utilities for data exchange between a model and a Geographical Information System (ie. GIS). In particular, model geographical, real and integer array data can be exported to ARCINFO and MAPINFO through “generate” and “mif/mid” files respectively. Model real and integer array data can be read as tables, allowing GIS-exported real and integer array data to be incorporated into a model.

An extremely important role performed by many of the Groundwater Data Utilities is the provision of assistance in model parameter definition, and in calculating the model-generated equivalents to field observations of head and flow. These, in conjunction with other utilities which automate the construction of input files for PEST (Doherty, 1994; Doherty, 2001a), facilitate the use of nonlinear parameter estimation techniques in the calibration of groundwater models. Other utilities are designed to enhance the parameter estimation capabilities of MODFLOW-2000, and assist in the provision of a data interface between MODFLOW-2000 and PEST.

None of the Groundwater Data Utilities are able to read database files. However many of them have been written to extract or process data of the type normally held in databases. To save programming effort and maintain independence from any particular database or platform, the utilities have been written to interface with “flat” ASCII files of a type that can be easily downloaded from a user’s groundwater database. In most cases, creation of a file type which adheres to the conventions used by the Groundwater Data Utilities can be achieved with little difficulty.

1.3 Installation Instructions

The Groundwater Data Utilities are distributed as a set of self-extracting archive files. Copy files GWUTILS1.EXE, GWUTILS2.EXE and GWUTILS3.EXE to a suitable directory on your hard disk (eg. C:\GWUTILS). Then run each of these executables in turn (by successively typing their names at the screen prompt) in order to extract and decompress the executable versions of the Groundwater Data Utilities. Then delete GWUTILS1.EXE, GWUTILS2.EXE and GWUTILS3.EXE in order to save disk space. When you have finished this process add the name of the utilities' directory to the PATH environment variable and reboot your machine.

QDIGIT, a shareware digitising program, can be installed from its self-extracting archive file QDG206.EXE in a similar manner. Similarly, the source code for the Groundwater Data Utilities is contained in the self extracting archive file SOURCE.EXE; source code files can be extracted by typing SOURCE once this file has been copied to a suitable subdirectory on your hard disk.

1.4 Source Code and Execution Details

Source code is provided for all of the Groundwater Data Utilities. All of the Utilities are written in (almost) ANSI Standard FORTRAN 90; thus, theoretically, they can be compiled to run on any platform for which a FORTRAN 90 compiler is available. Makefiles for use with the Lahey LF90 and LF95 compilers are included in the source code self-extracting archive file SOURCE.EXE. This file can be easily modified for use with other compilers on other platforms.

1.5 Features in Common

Though each of the programs comprising the Groundwater Data Utilities performs its own specific aspect of groundwater model pre- and/or postprocessing, all of the utilities share some common characteristics. Each requires that the user supply information in response to command-line prompts. While this can be a cumbersome method of communication between a program and its user, inconvenience has been mitigated somewhat by the fact that a user can always “backtrack” in program execution by entering “e” (for “escape”) at any prompt. Thus, whether a text string or number is expected, a simple “e” will cause the program to display its previous prompt; responding to this prompt with another “e” will make the program display the prompt before that, etc. Hence if, in the process of replying to a succession of screen prompts, incorrect data is entered at any stage, a user can “wind the program back” to the point at which previous data entries were all correct, and recommence execution from that point.

Most of the utilities read input files. Most perform exhaustive checking of these input files as they are read, documenting the line numbers and types of errors (if any) contained therein.

When undertaking model pre- and postprocessing using the Groundwater Data Utilities, certain files need to be read again and again. To ease the tedium of having to provide the names of one or more of these files each time a utility executes, their names can be placed into a “filename file” residing in the directory from which the utilities are run (ie. the “current directory”); this file must be named `files.fig` (note lower case in UNIX environment). Each utility tries to read `files.fig` from the current directory as soon as it commences execution. If it finds `files.fig` and reads it without error, the utility provides the user with default filenames (read from `files.fig`) when prompting him/her for the names of certain files. In each case the user can then either accept the default (as read from `files.fig`) or enter an alternative filename. Example 1.1 shows a filename file.

```
grid_specification_file=ex.spc
bore_coordinates_file=bores.crd
bore_sample_file=elev2.dat
bore_pumping_file=pump1.dat
pilot_points_file=points.dat
```

Example 1.1 A filename file.

A filename file can contain up to five lines of data, each line containing two items. The first is the name of a particular file type (with an underscore substituted for the space between words) while the second identifies the pertinent file. Note that full paths can be included in filenames. Note also that filenames containing spaces should be surrounded by quotes.

At present, only five types of file can be included in a filename file; these are easily identified in Example 1.1. These file types were chosen for inclusion as there is likely to be only one file of each of these types required over the entirety of a modelling exercise. Other commonly used file types (such as the bore listing file) were not chosen for inclusion in the filename file as different files of these types are likely to be required depending on the type of pre- or postprocessing being undertaken.

A particular type of file that must reside in the directory from which the Groundwater Data Utilities are run is a “settings file”. A settings file must be named `settings.fig` (note lower case in the UNIX environment). **Unlike the filename file whose presence is not essential, it is obligatory for a settings file to be present if certain of the utilities are to run;** if any of these utilities are invoked when a settings file is not present, the respective program will terminate execution with an appropriate error message. The utilities that require the presence of a settings file are those that read and/or write date and time information and those that read and/or write MODFLOW-compatible real and integer arrays. An example of a settings file is shown in Example 1.2

```
date=dd/mm/yyyy
colrow=yes
```

Example 1.2 A settings file.

One of the two possible lines contained in a settings file (the first in Example 1.2), informs the utilities of the date protocol to use in all input/output files, and in keyboard and screen interaction with the programs. In Example 1.2, the day precedes the month; the alternative is “mm/dd/yyyy”, in which case the month precedes the day. The other entry informs the utilities of the convention to use for formatted MODFLOW-compatible real and integer array storage. If `colrow` is set to “yes”, those utilities which read such arrays expect the array to be preceded by a header containing two numbers, viz. the number of columns and rows (in that order) comprising the finite difference grid. If `colrow` is set to “no”, such a header is not expected. Those utilities which generate MODFLOW-compatible real and integer arrays observe the same protocol when writing these arrays to a file. See Section 2.10 and 2.16 for further details.

1.6 Unformatted Files

Unfortunately, unformatted files generated by programs compiled by different FORTRAN compilers are not always interchangeable. It is thus possible that those of the utilities which read unformatted MODFLOW and/or MT3D output will not be able to read files generated by versions of these models compiled by certain FORTRAN compilers. If this occurs, contact me and I will send you a version of these programs that will read files generated by your particular model.

1.7 This Manual

This manual is divided into two parts. Part A, this part, provides an overview of the Groundwater Data Utilities and discusses aspects common to all of them. Part B documents each utility individually.

2. File Types

2.1 Introduction

This section lists the types of files used by the Groundwater Data Utilities. Most of the Utilities read one or more of, and/or generate one or more of, the types of files listed within this section.

Part B of this manual describes the Groundwater Data Utilities on a program-by-program basis. Within the program descriptions of Part B many references are made to the file types documented below.

2.2 Bore Coordinates File

A bore coordinates file lists bore identifiers, bore coordinates and, optionally, the model layer number pertaining to each bore. Example 2.1 shows part of a bore coordinates file.

13500002A	432757.001	7251364.668	1
13500002B	432532.650	7251332.776	2
13500005A	431938.751	7252252.603	1
13500006A	432189.994	7252530.667	1
13500007A	431794.596	7253020.996	1
13500008A	431852.452	7252682.867	1
13500009A	431992.097	7252806.516	1
13500012A	430844.466	7252185.675	1
13500015A	431043.509	7251663.817	1
13500017A	432970.533	7253641.892	1
13500023A	432885.506	7253795.232	1
13500032A	430646.701	7252430.711	1
13500032B	430700.251	7252953.946	2
13500032C	431519.999	7251789.264	3
13500042A	432406.371	7254192.785	1
13500047A	432185.152	7253514.981	1
13500049A	432018.367	7253175.856	1
13500050A	432184.395	7253668.732	1
13500052A	427669.234	7258198.290	1
13500053A	427556.282	7258320.658	1
13500054A	426825.900	7258378.399	1
13500055A	426378.631	7258006.921	1
13500056A	424855.152	7259321.369	1

Example 2.1 Extract from a bore coordinates file.

Each line of a bore coordinates file should possess at least three items. The first item is a bore identifier; this should consist of a maximum of 10 characters. For the Groundwater Data Utilities the bore identifier is case insensitive, being converted internally to upper case by each utility.

The second and third items on each line of a bore coordinates file consist of the east and north (ie. x and y) coordinates of the bore whose identifier comprises the first item on the line. The optional fourth item should be an integer indicating the model layer number to which the bore pertains. Many of the Groundwater Data Utilities do

not require that the fourth (layer number) column be present in a bore coordinates file. However for those programs that require a bore's layer number, the fourth column is essential.

Bores can be listed in any order in a bore coordinates file. However a bore coordinates file must not reference the same bore twice.

2.3 Bore Data File

A bore data file lists time-dependent borehole measurements in a form ready for use by the PEST MODFLOW/MT3D Utilities (Doherty, 1995) in preparing for MODFLOW or MT3D calibration using PEST. Note that as the PEST MODFLOW/MT3D Utilities have been largely superseded by the programs documented herein, use of this file type is rarely necessary. Example 2.2 shows part of a bore data file.

13500002A	30.0	26.50	1.0	h1
13500002A	60.0	27.00	1.0	h2
13500002A	90.0	27.04	1.0	h3
13500002A	120.0	20.57	1.0	h4
13500002A	150.0	20.07	1.0	h5
13500002A	180.0	20.03	1.0	h6
13500010A	30.0	26.44	1.0	h7
13500010A	60.0	26.94	1.0	h8
13500010A	90.0	26.97	1.0	h9
13500010A	120.0	20.56	1.0	h10
13500010A	150.0	20.07	1.0	h11
13500010A	180.0	20.03	1.0	h12
13500015A	30.0	26.37	1.0	h13
13500015A	60.0	26.86	1.0	h14
13500015A	90.0	26.90	1.0	h15
13500015A	120.0	20.55	1.0	h16
13500015A	150.0	20.07	1.0	h17
13500015A	180.0	20.03	1.0	h18
13500016A	30.0	26.33	1.0	h19
13500016A	60.0	26.81	1.0	h20
13500016A	90.0	26.85	1.0	h21
13500016A	120.0	20.55	1.0	h22
13500016A	150.0	20.07	1.0	h23

Example 2.2 Part of a bore data file.

Each line of a bore data file contains five entries. The first is the bore identifier, which must be of 10 characters or less in length. The next item on each line is the elapsed simulation time. This elapsed time must agree to within one part in 100000 with an elapsed time represented on a MODBORE or MT3BORE (programs of the PEST MODFLOW/MT3D Utilities) output file if the accompanying measurement is to be used in model calibration. Then follow the measurement and weight pertaining to the simulation time as well as the observation name to be used by PEST.

In building a bore data file it is important to observe the following rules:

- All weights must be either zero or positive; they cannot be negative.
- Observation names must be eight characters or less in length; they must also be unique.

Note that the order in which field borehole observations are listed in a bore data file is unimportant. Borehole measurements can be grouped by time, borehole or neither. For further details see the PEST MODFLOW/MT3D Utilities manual.

2.4 Bore Information File

A bore information file supplies information about one or more bores. A bore coordinates file (see Section 2.2) is one specific instance of a bore information file. Example 2.3 shows part of another bore information file.

13500002A	23.42	1.43e-4
13500002B	34.34	2.43e-3
13500005A	27.45	3.00e-3
13500006A	15.34	1.09e-2
13500007A	19.45	9.43e-3
13500008A	23.43	6.43e-3
13500009A	14.56	9.32e-4
13500012A	15.76	1.43e-2
13500015A	39.43	1.02e-2
13500017A	33.76	7.53e-3
13500023A	32.87	6.32e-3
13500032A	29.02	1.34e-2
13500032B	31.43	9.93e-4
13500032C	27.67	7.65e-3
13500042A	28.29	6.34e-3
13500047A	23.67	2.39e-3
13500049A	41.83	1.43e-4
13500050A	34.98	2.43e-3
13500052A	35.84	2.84e-3
13500053A	28.93	7.43e-5
13500054A	37.65	8.87e-3
13500055A	20.59	3.94e-3

Example 2.3 Extract from a bore information file.

Each line of a bore information file should possess at least two items. The first item is the bore identifier, an ASCII string of 10 characters or less in length. For the Groundwater Data Utilities the bore identifier is case-insensitive, all identifiers being converted to upper case internally.

Subsequent items on each line of a bore information file record different types of information pertaining to each bore. In Example 2.3 the second column records measured water elevations while the third column contains pollutant concentrations; all measurements pertain to samples gathered at the one time (or nearly the one time), thus constituting a “snapshot” of aquifer conditions. Items within each line may be separated by whitespace (including tabs) or a comma. Each line should contain the same number of items in order to maintain column consistency throughout the file.

It is important to note that a bore information file should not cite any bore more than once. Hence bore pumping files (Section 2.6) and bore sample files (Section 2.7) are not bore information files.

2.5 Bore Listing File

A bore listing file simply provides a list of bores, one to a line. Example 2.4 shows part of such a file.

```
13500002A
13500002B
13500005A
13500006A
13500007A
13500008A
13500009A
13500012A
13500015A
13500017A
13500023A
13500032A
13500032B
13500032C
13500042A
13500047A
13500049A
13500050A
13500052A
13500053A
13500054A
13500055A
```

Example 2.4 Extract from a bore listing file.

Different bore listing files are often used in conjunction with a single bore coordinates file, thus providing a mechanism whereby a subset of the latter can be selected for a particular type of groundwater data processing. Thus whenever a program reads both a bore coordinates file and a bore listing file, an error condition will arise if bores listed in the latter file are not also cited in the former file. However the reverse is not the case.

A bore listing file may possess more than one data column. If it does, only the first item on each line is read. Thus a file supplied to a program as a bore coordinates file can also be supplied to the same program as a bore listing file if it is desired that all bores in the former file be subject to processing of the type carried out by that utility.

For the Groundwater Data Utilities documented in this manual bore identifiers are case insensitive, being translated internally to upper case.

No bore should be cited more than once in a bore listing file. If it is, an error condition will arise and an appropriate error message will be displayed.

2.6 Bore Pumping File

A bore pumping file records the history of borehole extraction within a study area. Example 2.5 shows a fragment of such a file.

40050	20/06/1989	12:00:00	18/09/1989	12:00:00	0.000
40050	18/09/1989	12:00:00	18/12/1989	12:00:00	13.00
40050	18/12/1989	12:00:00	20/03/1990	12:00:00	65.00
40050	20/03/1990	12:00:00	27/06/1990	12:00:00	2.000
40050	27/06/1990	12:00:00	25/09/1990	12:00:00	3.000
40050	25/09/1990	12:00:00	20/12/1990	12:00:00	41.00
40050	20/12/1990	12:00:00	26/03/1991	12:00:00	58.00
40050	26/03/1991	12:00:00	25/06/1991	12:00:00	34.00
40050	25/06/1991	12:00:00	29/09/1991	12:00:00	25.00
40050	29/09/1991	12:00:00	09/01/1992	12:00:00	25.00
40050	09/01/1992	12:00:00	12/03/1992	12:00:00	35.00
40050	12/03/1992	12:00:00	26/06/1992	12:00:00	6.000
40050	26/06/1992	12:00:00	14/09/1992	12:00:00	0.000
40050	14/09/1992	12:00:00	04/01/1993	12:00:00	23.00
40051	04/01/1988	12:00:00	18/03/1988	12:00:00	13.00
40051	18/03/1988	12:00:00	15/06/1988	12:00:00	0.000
40051	15/06/1988	12:00:00	16/09/1988	12:00:00	2.000
40051	16/09/1988	12:00:00	28/10/1988	12:00:00	0.000
40051	28/10/1988	12:00:00	22/11/1988	12:00:00	3.000
40051	22/11/1988	12:00:00	04/01/1989	12:00:00	0.000
40051	04/01/1989	12:00:00	25/01/1989	12:00:00	0.000
40051	25/01/1989	12:00:00	21/02/1989	12:00:00	10.00

Example 2.5 Extract from a bore pumping file.

Each line of a bore pumping file must contain 6 entries. The first entry is the bore identifier which must be of 10 characters or less in length. When read by programs of the Groundwater Data Utilities the bore identifier is case-insensitive, being converted internally to upper case. (Note that coordinates corresponding to these bores will generally reside in an accompanying bore coordinates file; see Section 2.2 of this manual.) The next two items on each line of a bore pumping file define the starting date and time of a pumping interval. Depending on the contents of the settings file `settings.fig` (see Section 2.19), the date must be presented either in the format `dd/mm/yyyy` or `mm/dd/yyyy`; time must be recorded in the format `hh:mm:ss`. The next two items denote the end of a pumping interval using the same notation. The final item on each line lists the amount of pumping that has taken place during the nominated time interval; units are arbitrary.

The following rules must be observed when generating a bore pumping file:

- On any line of a bore pumping file the first date/time must precede the second date/time (ie. the first date must precede the second date or, if the dates are the same, the first time must precede the second time).
- For the same bore, the first date and time on any given line of a bore pumping file must be the same as the second date and time on the previous line.
- All entries pertaining to any given bore must follow one after the other (in temporal sequence, as noted above); a sequence of entries for a certain bore must not be interspersed with a sequence of entries for another bore.

In most cases a bore pumping file will have been either downloaded from a user's groundwater database or constructed from a file downloaded from such a database. Where a modeller is working in an area of high groundwater usage, the bore pumping file may be very large. While this poses no problem to members of the Groundwater Data Utilities suite, there is a software-imposed limit to the number of entries

permitted for a single bore. In all cases this limit is easily adjusted by making a minor source code alteration. The nature of this alteration will be provided as an appropriate error message in the unlikely event of its being required.

Both positive and negative pumping figures are permitted in the final column of the bore pumping file.

2.7 Bore Sample File

A bore sample file records data gathered at discrete sample times at a number of specific locations, eg. water level or chemical concentration data gathered through borehole sampling programs. Each line of a bore sample file has four, possibly five, entries, each of which must be separated from its neighbouring entry by one or more whitespace (including tab) characters. Typically a bore sample file will hold data extracted from a groundwater database. There is no limit to the size of this file as all Groundwater Data Utility programs which read it hold only part of its contents in memory at any one time. However there is a limit to the maximum number of entries allowed for any one bore. This limit is easily adjusted by making a slight alteration to pertinent source code files. The nature of this adjustment will be provided as part of an appropriate error message in the unlikely event of its being required. Example 2.6 shows part of a bore sample file.

13500002A	25/09/1991	12:00:00	12.00	
13500002A	02/01/1992	12:00:00	11.83	
13500002A	24/03/1992	12:00:00	12.81	
13500002A	29/06/1992	12:00:00	13.54	
13500002A	22/09/1992	12:00:00	13.24	
13500002A	17/12/1992	12:00:00	12.84	
13500002A	22/03/1993	12:00:00	12.38	x
13500002A	21/06/1993	12:00:00	11.83	x
13500002A	27/09/1993	12:00:00	11.61	x
13500002A	16/12/1993	12:00:00	12.35	
13500002A	01/03/1994	12:00:00	11.79	
13500002A	22/03/1994	12:00:00	11.89	
13500005A	19/02/1959	12:00:00	29.84	
13500005A	05/03/1959	12:00:00	30.33	
13500005A	20/03/1959	12:00:00	30.76	
13500005A	06/04/1959	12:00:00	31.19	
13500005A	17/04/1959	12:00:00	31.45	
13500005A	01/05/1959	12:00:00	31.65	
13500005A	15/05/1959	12:00:00	31.65	
13500005A	29/05/1959	12:00:00	31.65	
13500005A	12/06/1959	12:00:00	31.65	
13500005A	26/06/1959	12:00:00	31.46	
13500005A	10/07/1959	12:00:00	31.34	

Example 2.6 Extract from a bore sample file.

The first item on each line of a bore sample file is a bore identifier. This identifier must be of 10 characters or less in length. When used with programs of the Groundwater Data Utilities the bore identifier is case-insensitive. The second item is the date; depending on the contents of the settings file `settings.fig`, this must be expressed either in the format `dd/mm/yyyy` or `mm/dd/yyyy`. Then follow the time (in the format `hh:mm:ss`) and the borehole measurement pertaining to the cited

date and time. An optional fifth item may be present on any line; if present this item must consist solely of the single character “x” to indicate that the previous data element lacks integrity (for example if a borehole water elevation measurement must be treated with suspicion because it is suspected that the bore was dry).

The following rules must be observed when generating a bore sample file:

- For any one bore, dates and times must be listed in increasing order.
- All entries for the same bore must be in juxtaposition; in other words, it is not permitted to list some of the entries for a particular bore in one part of a bore sample file and the remainder of the entries in another part of the same file, with data pertaining to one or more other bores in between.

As most groundwater data is sampled at a measurement interval that far exceeds one day, measurement time-of-day is rarely recorded in the field. Thus a “notional” measurement time (for example midday as shown in Example 2.6) can be attributed to all samples.

2.8 Filename File

As explained in Section 1.5, a filename file (which must possess the name `files.fig`) contains the names of files which are likely to be repeatedly read by programs of the Groundwater Data Utilities. When a program requiring the name of such a file is run, the pertinent filename, as read from the filename file, is displayed in square brackets following the prompt. The user may then either press the <Enter> key to accept the default or type in the correct filename him/herself.

As shown in example 2.7 below, only five types of file can currently be represented in a filename file. These can be listed in any order. References to any of these files can be omitted from the filename file if desired. Note also that if a filename contains a space, it should be enclosed in quotes.

```
grid_specification_file=ex.spc
bore_coordinates_file=bores.crd
bore_sample_file=elev2.dat
bore_pumping_file=pump.dat
pilot_points_file=points.dat
```

Example 2.7 A filename file.

The file types listed in Example 2.7 were selected for inclusion in the filename file because different members of the Groundwater Data Utilities are likely to repeatedly access these same files. Thus, for example, a bore coordinates file can list the coordinates of all bores found within a certain project area; different bores can be selected for different types of pre- and postprocessing using different bore listing files. Similar considerations apply to the bore sample file and the bore pumping file. The grid specification file is likely to be unique to a particular project area.

Use of a filename file is optional. If present it will only be read by a member of the Groundwater Data Utilities if it resides in the directory from which that utility was

run. If absent, a Groundwater Data Utility will not display a default filename in brackets when prompting the user for the name of any of the types of file listed in Example 2.7.

2.9 Grid Specification File

A grid specification file contains all of the information required to draw the finite difference grid on a map using real-world coordinates. Thus information contained in this file can be used to determine the positions of bores with respect to the grid, superimpose model outcomes on other geographical data, and much more. Many of the Groundwater Data Utilities begin execution by reading a grid specification file. Some of the utilities simply need to read the grid dimensions while others need to know the full complement of geographical information encompassed in the grid design. Example 2.8 shows the grid specification file for a small grid consisting of 8 rows and 10 columns. Fig. 2.1 shows the grid to which it pertains.

```
8 10
300000.0 7800000.0 30.0
2*100 6*50 2*100
50 50 50 50 50 50 50 50
```

Example 2.8 A grid specification file.

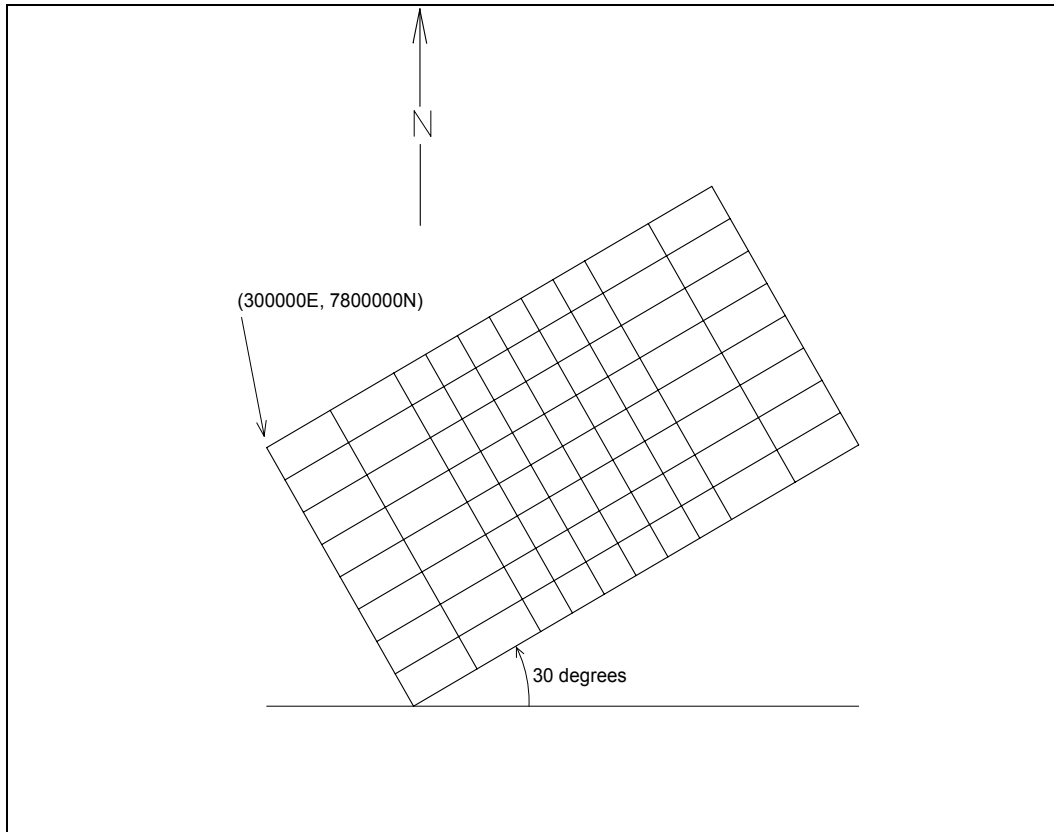


Figure 2.1 The finite difference grid whose grid specification file is shown in Example 2.8

Each line of a grid specification file contains two or more items; each item must be separated from its neighbours by a space, comma or tab. The first line contains two items, viz. the number of rows and columns respectively, within the finite-difference grid. (It should be noted that, where it is used, the header to a formatted, MODFLOW-compatible, real or integer array contains these grid dimensions in reverse order, the result of an unfortunate historical accident.) Use, or otherwise, of this header in formatted array storage is determined by the `colrow` setting in the “settings file”, `settings.fig`; see Section 2.19 for further details.

The second line of a grid specification file is comprised of three entries. These are the east and north (ie. x and y) coordinates of the top left corner of the finite difference grid, and the rotation of the grid row direction with respect to east (positive for anticlockwise, negative for clockwise); see Fig. 2.1. This angle must be expressed in degrees and must lie between -180 and 180 degrees.

The third line of a grid specification file holds the MODFLOW *delr* vector. This is a list of grid row widths in order of increasing column index. There should be as many entries in this vector as there are columns in the finite difference grid. Note that it is not necessary to write all elements of the *delr* vector on the one line if the line

becomes too long. All programs which read a grid specification file will continue reading subsequent lines until enough elements have been read.

Next, on a new line, follows the MODFLOW *delc* vector, ie. a list of grid cell widths in the column direction; the number of such entries must equal the number of rows comprising the finite-difference grid. As with the *delr* vector, elements can wrap around to the next line if desired.

Example 2.8 demonstrates a shorthand method by which cell row and column widths can be supplied in the grid specification file. Using this method, a list of n identical entries of magnitude b can be replaced by the term $n*b$.

2.10 Integer Array File

As the name implies, an integer array file holds a MODFLOW/MT3D-compatible integer array. Such a file can be formatted or unformatted, the latter being a form of binary data storage which, in general, conserves disk space. The protocol for storing unformatted integer array files is such that they are capable of being read by the MODFLOW utility subroutine U2DINT which possesses an unformatted read option.

A formatted integer array can be software-generated or written manually using a text editor. Example 2.9 shows the contents of a small integer array file.

10	8								
3	3	3	3	3	3	3	4	4	4
3	3	3	3	3	3	4	4	4	4
2	3	3	3	3	4	4	4	4	4
2	2	2	3	4	4	4	4	4	4
2	2	2	2	2	5	5	5	5	5
2	2	2	5	5	5	5	5	5	5
2	2	2	5	5	5	5	5	5	5
2	2	2	2	2	5	5	5	5	5

Example 2.9 A formatted integer array file.

The first line of a formatted integer array file contains two entries, viz. the number of columns and rows, respectively, in the model finite-difference grid. Note that these two quantities are listed in reverse order to their appearance in a grid specification file. *Note also that if `colrow` is set to “no” in the settings file `settings.fig`, then this line must be omitted.*

Next follows the integer array. The array is listed row by row starting from the top of the grid. $ncol$ integers must be supplied for each row, where $ncol$ is the number of columns in the finite-difference grid. The listing of row elements can wrap around onto the next line if necessary; however the elements of each new row must begin on a new line. Individual elements must be separated by spaces, tabs or a comma.

Those Groundwater Data Utility programs which write integer arrays do so using the FORTRAN format specifier “(20I5)”. To maintain whitespace between array elements their values must lie between -999 and 9999.

Any Groundwater Data Utility that reads or writes an integer array first inquires of the user the name of the file in which the array resides or to which it must be written. If the filename so supplied possesses an extension of “INF”, the utility assumes that the file is formatted (“INF” stands for “INteger Formatted”). However if the user supplies a filename with an extension of “INU” the relevant file is assumed to be unformatted (“INU” stands for “INteger Unformatted”). If the supplied filename possesses a different extension from both of these, the user is asked specifically whether the file is formatted or unformatted so that it can read or write the file in the appropriate manner.

2.11 Integer Array Table File

An integer array table file holds an integer array written in tabular form. It holds either two or three columns of data. The first two items on each line of a three-column integer array table file list a cell row and column number respectively. The third item holds the integer array value pertaining to the cell whose row and column numbers comprise the previous entries on the line. Line entries can be tab, space or comma-delimited. Example 2.10 shows part of an integer array table file.

21	24	1
21	25	1
21	26	1
21	27	1
21	28	1
21	29	6
21	30	6
21	31	6
21	32	6
21	33	6
21	34	6
21	35	6
21	36	6
21	37	1
21	38	1
21	39	1
21	40	1
21	41	1
21	42	1
21	43	1
21	44	1
21	45	1

Example 2.10 Extract from a three-column integer array table file.

As the name implies, each line of a two-column integer array table file possesses two items. The first item on each line is a cell number whereas the second item is the integer array value pertaining to the cell whose cell number appears as the first line item. A cell number is a means of cell identification obtained by counting cells row by row from the top left of the finite difference grid.

It is not necessary that every cell contained within a finite-difference grid be referenced in an integer array table file; those Groundwater Data Utilities which read such files supply a default value for missing elements.

The principal use of an integer array table file is in exchanging integer array data with a Geographical Information System (GIS). An integer array can be uploaded from a model to a GIS as, for example, a MIF/MID file combination, a three-column integer array table being housed in the MID file. In a GIS, array elements within this table (final column only) can be altered in accordance with geographical data contained within other information layers covering the same study area. Integer array data edited in this fashion can then be downloaded as a text file such as is shown in Example 2.10 and formatted as an integer array using pertinent Groundwater Data Utility programs.

2.12 Pilot Points File

A pilot points file is very similar to a bore coordinates file; however, in the case of a pilot points file, the integers in the fourth column refer to zones within a model domain rather than to layers. Furthermore, the file contains a fifth column listing data pertaining to each pilot point. Example 2.11 illustrates a pilot points file.

pp1	5045.644	5450.288	1	1.23
pp2	6481.347	4807	1	0.89
pp3	7455.778	5622.2	1	2.34
pp4	6809.895	6832.13	1	2.19
pp5	9629.16	6862.751	1	1.98
pp6	10443.17	6133.803	1	0.23
pp7	12172.05	6396.549	1	0.32
pp8	11806.35	7939.032	1	1.03
pp9	9517.249	4838.306	2	10.2
pp10	10430.28	4825.698	2	13.6
pp11	10583.86	3666.904	2	9.43
pp12	8686.321	3047.161	2	8.32
pp13	6894.65	3704.822	2	6.43
pp14	5620.683	2736.789	2	10.4

Example 2.11 A pilot points file.

The first entry on each line of a pilot points file is the “pilot point identifier”; like a bore identifier, this should be of 10 characters or less in length and is case-insensitive. Then follow the easting and northing of the pilot point. The next entry is an integer, this normally identifying the zone within a model domain in which spatial interpolation is affected by the value assigned to the pilot point; such zonation is normally defined by a MODFLOW-compatible integer array. The final entry on each line of a pilot points file is the value assigned to the pilot point. For those members of the Groundwater Data Utilities which read a pilot points file, these values are used for spatial interpolation to the cells of the finite difference grid.

Pilot points are a useful device for assigning properties to a model domain. As such, they are a useful complement to PEST’s predictive analysis and/or regularisation capabilities. When used in this way, data in the final column of a pilot points file may represent hydraulic conductivity or some other aquifer property.

Entries on each line of a pilot points file should be space or tab-delimited.

2.13 QDIGIT Contour File

QDIGIT is a shareware digitising program which can be used with many different digitisers. It records geographical information in a number of different formats, the format depending on the type of information being digitised. A “QDIGIT contour file” is the name given in this manual to the type of file in which it stores labelled line data; the option to digitise labelled line data is available through Digit's “Digitise/Contours” menu item. Example 2.12 shows part of such a file.

406402.72	7248411.42	300
406407.73	7248403.84	300
406412.76	7248398.79	300
406415.25	7248391.21	300
406420.28	7248386.16	300
406422.77	7248378.58	300
406427.80	7248373.53	300
406432.82	7248365.95	300
406437.85	7248360.90	300
406440.34	7248353.32	300
406445.37	7248348.27	300
406447.87	7248343.22	300
406450.37	7248338.16	300
406452.89	7248335.64	300
ENDLINE		
406455.40	7248333.11	300
406457.90	7248328.06	300
406460.42	7248325.53	300
406462.95	7248325.54	300
406462.93	7248323.01	300
406465.45	7248320.48	300
406465.45	7248320.48	300

Example 2.12 Extract from a QDIGIT contour file.

Each line of a QDIGIT contour file is comprised of three items. The first two items are point coordinates along the line; the third is the line label. The end of a line is marked by the single entry “ENDLINE”.

See Section 3 of this manual for a discussion of the use of QDIGIT both in model preprocessing and in preparing map data for display.

2.14 QDIGIT Line File

QDIGIT is a shareware digitizing program which can be used with many different digitisers. It records geographical information in a number of different formats, the format depending on the type of information being digitised. A “QDIGIT line file” is the name given in this manual to the type of file in which it stores digitised line data. Example 2.13 shows part of such a file.

400432.45	7250327.45
400456.18	7250327.85
400466.94	7250328.13
400474.83	7250328.89
400506.61	7250329.74
400524.97	7250329.73
400543.35	7250330.98
400550.86	7250330.09
400557.15	7250331.36
ENDLINE	
412090.06	7259658.74
412090.84	7259658.35
412090.89	7259659.85
412090.23	7259659.98
412090.53	7259659.32
412090.97	7259659.62
412090.14	7259660.98
412090.67	7259660.13
412090.63	7259661.86

Example 2.13 Extract from a QDIGIT line file.

QDIGIT records geographical line data as a set of coordinates along the line; each coordinate pair is written to a separate line. The end of each line is marked by the “ENDLINE” string in place of a coordinate pair.

See Section 3 of this manual for a discussion of the use of QDIGIT both in model preprocessing and in preparing map data for display.

2.15 QDIGIT Points File

QDIGIT is a shareware digitizing program which can be used with many different digitisers. It records geographical information in a number of different formats, the format depending on the type of information being digitised. A “QDIGIT points file” is the name given in this manual to the type of file in which it stores data digitised through the QDIGIT “Digitise/Points” option. Example 2.14 shows part of such a file.

407124.26	7255055.16
407809.80	7254497.42
407451.24	7253671.15
406592.95	7254503.79
410097.71	7258194.62
413410.89	7255574.70
407195.24	7256082.01
407810.22	7255081.70
408450.62	7254490.59
409226.45	7253988.22
407989.94	7253562.32
407237.83	7254502.06
406514.82	7255044.21
406718.95	7253925.61
405954.31	7253639.00
406787.48	7252980.51

Example 2.14 Extract from a QDIGIT points file.

Each line of a QDIGIT points file consists of two entries, viz. the coordinates of each digitised point. Note that such a file is immediately useable by SURFER as a basis for posting symbols on a map.

2.16 QDIGIT Well File

QDIGIT is a shareware digitizing program which can be used with many different digitisers. It records geographical information in a number of different formats, the format depending on the type of information being digitised. A “QDIGIT well file” is the name given in this manual to the type of file in which it stores digitised points data together with associated labels; data digitised through the QDIGIT “Digitise/Well Locations” option is stored in this form. Example 2.15 shows part of such a file.

407124.26	7255055.16	PROD1
407809.80	7254497.42	PROD2
407451.24	7253671.15	PROD3
406592.95	7254503.79	PROD4
410097.71	7258194.62	OBS1
413410.89	7255574.70	OBS2
407195.24	7256082.01	OBS3
407810.22	7255081.70	OBS4
408450.62	7254490.59	OBS5
409226.45	7253988.22	OBS6
407989.94	7253562.32	OBS7
407237.83	7254502.06	OBS8
406514.82	7255044.21	OBS9
406718.95	7253925.61	OBS10
405954.31	7253639.00	OBS11
406787.48	7252980.51	OBS12
403437.85	7250744.23	OBS13

Example 2.15 Extract from a QDIGIT well file.

Each line of a QDIGIT well file is comprised of three entries. The first two entries are a point’s coordinates while the third is the point’s label. Such a file is immediately useable by SURFER for posting labelled information on a map.

2.17 Real Array File

As the name implies, a real array file holds a MODFLOW/MT3D-compatible real array. Such a file can be formatted or unformatted, the latter being a form of binary data storage which, especially in the case of real arrays, conserves disk space. The protocol for storing unformatted real array files is such that they are capable of being read by the MODFLOW utility subroutine U2DREL. Note that unformatted file storage is compiler-specific. Thus an unformatted file written by a program compiled with a certain FORTRAN compiler may not be readable by a program compiled with another FORTRAN compiler; see Section 1.6 for more details.

A formatted real array, on the other hand, can be either software-generated or written manually using a text editor. Example 2.16 shows the contents of a small formatted real array file.

10	8						
3.567	3.567	3.567	3.567	3.567	3.567	3.567	4.539
4.539	4.539						
3.567	3.567	3.567	3.567	3.567	4.539	4.539	4.539
4.539	4.539						
2.34e-1	3.567	3.567	3.567	3.567	4.539	4.539	4.539
4.539	4.539						
2.34e-1	2.34e-1	2.34e-1	3.567	4.539	4.539	4.539	4.539
4.539	4.539						
2.34e-1	2.34e-1	2.34e-1	2.34e-1	2.34e-1	5.1	5.1	5.1
5.1	5.1						
2.34e-1	2.34e-1	2.34e-1	5.1	5.1	5.1	5.1	5.1
5.1	5.1						
2.34e-1	2.34e-1	2.34e-1	5.1	5.1	5.1	5.1	5.1
5.1	5.1						
2.34e-1	2.34e-1	2.34e-1	2.34e-1	2.34e-1	5.1	5.1	5.1
5.1	5.1						

Example 2.16 A formatted real array file.

The first line of a formatted real array file contains two entries, viz. the number of columns and rows, respectively, in the model finite-difference grid. Note that these two quantities are listed in reverse order to their appearance in a grid specification file. *Note also that if `colrow` is set to “no” in the settings file `settings.fig`, then this line must be omitted.*

Next follows the real array. The array is listed row by row starting from the top of the grid. *ncol* numbers must be supplied for each row, where *ncol* is the number of columns in the finite-difference grid. While the listing of row elements can wrap onto the next line if necessary, the first element of each new row must begin on a new line. Individual elements must be separated by spaces, tabs or a comma.

Any utility that reads or writes a real array first inquires of the user the name of the file in which the array resides, or to which it must be written. If the filename so supplied possesses an extension of “REF”, the utility assumes that the file is formatted (“REF” stands for “REal Formatted”). However if the user supplies a filename with an extension of “REU” the relevant file is assumed to be unformatted (“REU” stands for “REal Unformatted”). If the supplied filename possesses a different extension from both of these, the program asks the user specifically whether the file is formatted or unformatted so that it can read or write the file in the appropriate manner.

2.18 Real Array Table File

A real array table file holds a real array written in tabular form. It holds either two or three columns of data. The first two items on each line of a three-column real array table file list a cell row and column number respectively. The third item holds the real array value pertaining to the cell whose row and column numbers comprise the previous entries on the line. Line entries can be tab, space or comma-delimited. Example 2.17 shows part of such a real array table file.

21	24	1.3445
21	25	1.3445
21	26	1.3445
21	27	1.3445
21	28	1.3445
21	29	6.5641
21	30	6.5641
21	31	6.5641
21	32	6.5641
21	33	6.5641
21	34	6.5641
21	35	6.5641
21	36	6.5641
21	37	11.432
21	38	11.432
21	39	11.432
21	40	11.432
21	41	11.432
21	42	11.432
21	43	11.432
21	44	11.432
21	45	11.432

Example 2.17 Extract from a three-column real array table file.

As the name implies, a two-column real array table file possesses two columns of data. The first item on each line is a cell number whereas the second item is the real array value pertaining to the cell whose cell number appears as the first line item. A cell number is a means of cell identification obtained by counting cells row by row from the top left of the finite difference grid.

Note that it is not necessary that every cell contained within a finite-difference grid be referenced in a real array table file. Any Groundwater Data Utility program which reads such a file supplies a default value to uncited cells.

The principal use of a real array table file is in exchanging real array information with a Geographical Information System (GIS). A real array can be uploaded from a model as, for example, a MIF/MID file combination, a three-column real array being housed in the MID file; in a GIS the array elements within this table (final column only) can be altered in accordance with geographical data contained within other information layers covering the same study area. Real array data edited in this fashion can then be downloaded as a text file such as is shown in Example 2.17 and reformatted as a real array again using pertinent Groundwater Data Utility programs.

2.19 Settings File

A settings file must be present within any directory from which certain of the Groundwater Data Utilities are invoked. The utilities which require it are those that read and/or write date and time information and those which read and/or write MODFLOW-compatible real and/or integer arrays. A settings file, which must possess the name `settings.fig`, is illustrated in Example 2.18.

```
date=dd/mm/yyyy  
colrow=yes
```

Example 2.18 A settings file.

A settings file requires two lines, one informing the Groundwater Data Utilities of the protocol for expressing dates, and the other informing them of the convention to use for storage of formatted, MODFLOW-compatible, real and integer arrays. These lines can be written to the settings file in either order.

The first line appearing in Example 2.18 informs the utilities that, in expressing dates in all pertinent input and output files, as well as in all pertinent terminal and screen input/output, the date is to precede the month. However if the first entry in Example 2.18 were written as “date=mm/dd/yyyy”, then the month must precede the day in representations of date.

As was explained in Sections 2.10 and 2.17, formatted files containing real and integer arrays can optionally begin with a one-line header containing the number of columns and rows (in that order) in the finite difference grid. (This header is expected by certain commercial MODFLOW graphical user interfaces.) If `colrow` is set to “yes” in the settings file, then this header is expected on any real or integer array read by any member of the Groundwater Data Utility suite. Alternatively, if `colrow` is set to “no”, members of the Groundwater Data Utilities will expect formatted real and integer arrays to contain no such header, and will write formatted real and integer array files in which the header is omitted.

2.20 Structure File

A structure file stores geostatistical data pertaining to a model domain in the form of one or more variograms assigned to one of more “geostatistical structures”. Each such geostatistical structure can contain up to 5 nested variograms and a nugget. Each such structure is normally assigned to a particular zone within the model domain, different zones normally being differentiated from each other on the basis of different values in a model-compatible integer array.

Example 2.19 depicts a structure file.

```
STRUCTURE struct1
  NUGGET 0.0
  TRANSFORM log
  NUMVARIOGRAM 2
  VARIOGRAM var1 0.6
  VARIOGRAM var2 0.3
END STRUCTURE

VARIOGRAM var1
  VARTYPE 2
  BEARING 72
  A 3000
  ANISOTROPY 13.5
END VARIOGRAM

VARIOGRAM var2
  VARTYPE 1
  BEARING 72
  A 4000
  ANISOTROPY 5.0
END VARIOGRAM

STRUCTURE struct2
  NUGGET 0.0
  TRANSFORM none
  NUMVARIOGRAM 1
  MAXPOWERVER 10000
  VARIOGRAM var3 .005
END STRUCTURE

VARIOGRAM var3
  VARTYPE 4
  BEARING 20
  A 1.0
  ANISOTROPY 1.0
END VARIOGRAM
```

Example 2.19 A structure file.

A structure file is made up of any number of separate incidences of two different types of entity. These entities are the “structure” entity and the “variogram” entity. The latter entity specifies a variogram. Any number of such variograms can be nested to form a geostatistical structure. Kriging within each zone of the model domain, as carried out by programs such as PPK2FAC and FAC2REAL, is based on the geostatistical properties of an area as defined in a structure. Any number of structures and variograms can be cited in a structure file.

Complete specifications of a structure file are presented in the documentation to program PPK2FAC in Part B of this manual. See also Section 5 of the present document where the use of pilot points and geostatistical methods in model parameterisation and calibration is fully discussed.

2.21 Parameter Replacement File

A parameter replacement file is used by program FAC2MF2K which replaces some of the parameters occurring in an existing MODFLOW-2000 input dataset, by a new set of parameters based on pilot points. The contents of this file specify what parameters are to be removed from the MODFLOW-2000 input dataset and what parameters are to be added. Modifications to the MODFLOW-2000 *multiplier* and *zone* files can also be specified through this file.

Example 2.20 illustrates a parameter replacement file.

```
REPLACE  hk
  out hk_1
  out hk_2
  out hk_3
  out hk_5
  out hk_6
  newparamlays 1 2
#  newparamprefix "k_"
  transformtype log
  minparval 1e-2
  maxparval 1e3
#  mininterpval 1e-2
#  maxinterpval 1e3
  mininterpfile lowlim.ref
  maxinterpfile highlim.ref
END REPLACE

removezone  zhk1
removezone  zhk2
removezone  hk1
removemult  hk2
```

Example 2.20 A parameter replacement file.

Complete specifications for a structure file are presented in the documentation to program FAC2MF2K in part B of this manual. See also Section 5 of the present document where the use of pilot points and geostatistical methods in model parameterisation and calibration is fully discussed.

3. Working with QDIGIT

3.1 Introduction

QDIGIT is a shareware digitizing program that was obtained via the internet from the SimTel anonymous ftp site. It was written by Peter Jahans while he was at the University of Alberta. His new address is:

Peter C. Jahans
5599 San Felipe, Suite 1700
Houston, Texas 77056
USA
Email: pjahans@houston.geoquest.slb.com

Peter requests that anyone who, after an evaluation period, continues to use QDIGIT, forward him \$US50 as payment for the software. A WINDOWS graphical version is presently under development.

QDIGIT is capable of working with many different kinds of digitizer. It is easy to use, allowing for the recording of line (labelled and unlabelled), point (labelled and unlabelled) and outcrop data. Data is stored in ASCII files with easily-understood formats. Though designed for use in a geological context, it is extremely useful in a hydrogeological context as well. Documentation exists in the form of a QDIGIT.DOC file supplied with the software.

This section briefly discusses some of the processing options available for QDIGIT-generated files. It also makes mention of an idiosyncrasy of QDIGIT that could result in the production of very long output files if a user is not wary, and discusses how such files can be “cleaned” by the processing facilities available through the Groundwater Data Utilities suite.

3.2 Points File

Example 2.14 shows an extract from a QDIGIT points file. This is the file produced when a user selects the “Points” option from the “Digitize” menu. When digitizing in “points” mode a user can click on any number of points in succession; as he/she does so, QDIGIT writes the coordinates of the digitized points to a file. Note that, as is explained in the QDIGIT documentation, QDIGIT never overwrites a file; if a user supplies a pre-existing filename for digitized data storage, the newly-digitized data is appended to that file.

A points file is immediately useable by mapping and GIS software for the plotting of point coordinates as user-selected symbols. Alternatively, the Groundwater Data Utility QDIG2DXF can produce a DXF file on the basis of a QDIGIT-generated points file by representing each point as a cross (ie. two intersecting lines) of user-specified length, this length being specified in map units.

Note that QDIGIT is not alone in representing point data in the format illustrated in Example 2.14; a similar file can be generated using the SURFER “digitize” option. Such a file could also be produced by “manually” digitizing data, ie. by typing point coordinates directly into a text file using a text editor. In all of these cases QDIG2DXF can be used to generate a DXF file suitable for importation into model graphical user interface packages.

3.3 Well File

A QDIGIT-generated well file is illustrated in Example 2.15. It is similar to a points file in that its first two data columns list digitized point eastings and northings. However it contains an additional third column containing point labels. These labels are typed into QDIGIT by the user as each point is digitized.

A QDIGIT well file is immediately useable by most mapping and GIS software for plotting and labelling of point data. If desired, points can also be plotted as scaled symbols, the size of the symbol depending on numbers in the final column of the well file if this column contains numeric data.

Program QDIG2DXF from the Groundwater Data Utilities can be used to produce a DXF file on the basis of the data contained in a QDIGIT well file. QDIG2DXF manages a well file in exactly the same way that it manages a points file, producing a cross of user-specified length in DXF format corresponding to every point in the file; the label column is ignored. A DXF file produced in this fashion by QDIG2DXF can be read by graphical model preprocessors (which generally require geographical data in DXF format) in order to provide a map underlay to model data.

3.4 Line File

When the “Lines” option of the “Digitize” menu is selected QDIGIT instructs the user on how to digitize lines on a map. It says, “Hold down button while tracing lines. Press <Enter> to signal the end of a line segment.” QDIGIT allows a user to record data pertaining to many line segments in a single file; to terminate file output press the <Esc> key. Example 2.13 shows part of a QDIGIT-generated line file. Each recorded line segment consists of a sequence of point eastings and northings; the “ENDLINE” string marks the end of a particular line segment.

It is important to understand the operation of QDIGIT when digitizing line data. When used with certain types of digitizer QDIGIT writes coordinates information to its line file at a faster rate than this information is supplied to it by the digitizer. While it is awaiting new information from the digitizer QDIGIT repeatedly writes the coordinates of the last digitized point to its output file. When more information arrives from the digitizer, QDIGIT then proceeds to continuously write the newly-acquired point coordinates to its output file, and so on. As a result of this process, a QDIGIT line file can become very large. A user is advised that once he/she presses the digitizer’s button to begin continuous digitization of a line, he/she should proceed

as quickly as possible. When the end of the line has been reached, press <Enter> immediately so that QDIGIT ceases to write information to its output file. (A user can then rest between digitizing separate line segments.)

An alternative to continuous line digitization is to digitize lines in straight segments. This method is appropriate for items such as roads and railway lines that consist of linked straight sections. In this mode of operation a user should only press the digitizer button where the road or railway line bends, ie. at points that mark the beginning of one segment and the end of another. However, for certain digitizers, QDIGIT continues to frantically write points to its output file even when the digitizer button is not depressed, the recorded coordinates being those corresponding to the last point at which the digitizer button was pressed. Hence, even when lines are digitized in this point-by-point mode, the operation should proceed as quickly as possible, and no time should be wasted before pressing the <Enter> key to mark the end of a particular line.

It is apparent from the above discussion that when used to digitize lines, QDIGIT can write a large amount of redundant information to the “line file” which it produces. For most applications this redundant information must be removed.

Because a QDIGIT line file consists of a column of eastings and a column of northings, most mapping packages can read it directly and display points along the line as symbols on a map (the package must be capable of ignoring the “ENDLINE” strings which separate different lines). However in most cases a user will require that digitized line data be plotted as lines. While it is not difficult to edit a QDIGIT line file manually to reformat it as a SURFER blanking file (which can be plotted as line data or used to blank out part of a contour grid), a faster method to convert line data into a more readily useable form is to use program QDIG2DXF to rewrite the line data in DXF format.

When used to translate QDIGIT line data to DXF format, QDIGIT asks the user for an appropriate “trimming distance”. This is roughly the distance, in map units, for which QDIGIT will write consecutive points in the DXF file which it generates. Note that it is only a rough guide to ultimate vertex separation on the QDIG2DXF-generated DXF output file for QDIG2DXF does not calculate the exact distance between each pair of points to decide whether or not to reject a particular point. Instead, to save execution time, it calculates the difference between subsequent *x* and *y* coordinates as a lower bound on the actual point separation. Thus neighbouring vertices can be much closer on the DXF file produced by QDIG2DXF than the user-supplied trimming distance; however they will never be greater than the trimming distance apart.

When a line is digitized in the point-by-point mode described above for roads and railways, it is wise to supply a very small trimming distance. Though point-by-point line files produced by QDIGIT may be large because of the multifold repetition of points on which the digitizer button is pressed, these redundant points are easily eliminated as they are separated from previous points by zero distance. Thus if a trimming distance is supplied which is less than the minimum distance between

successive corners and greater than zero, all redundant information will be winnowed by QDIG2DXF from the line file, and all corners will be preserved.

3.5 Contour File

Contours are digitized in a similar manner to lines. However QDIGIT requires that a user provide a label (normally a contour elevation) for each line. Lines are digitized one by one, QDIGIT requiring a filename for each labelled line. By entering the same filename for each such labelled line, all contour line data will be recorded in the same file (because QDIGIT never overwrites a file; it always appends to it). Similar considerations to those outlined above for digitizing unlabelled lines apply to digitizing contour lines, ie. lines must be digitized fast when using certain digitizers to circumvent the production of excessively large files holding an abundance of redundant information.

Like a line file, a QDIGIT contour file can be read as a points file and used to plot individual points along each line (with or without labelling information); however this is not a common use for such files. They can also be read as line files; QDIG2DXF can be used to reformat labelled line data into polyline DXF format for subsequent display using model preprocessing and/or mapping software. However the Groundwater Data Utilities provide a further option for the processing of contour line data acquired by QDIGIT. Program QDIG2XYZ is able to read QDIGIT-generated contour lines and produce *xyz* data files for the use of contouring/gridding programs such as SURFER. In this way the elevation information content of a contour map can be used to produce a gridded dataset or digital elevation model.

Like QDIG2DXF, QDIG2XYZ requires that the user supply a “trimming” distance, the role of which in QDIG2XYZ is similar to its role in QDIG2DXF, ie. it provides a rough criterion for the eradication of unwanted data based on separations between successively digitized points.

4. Some Common Tasks

4.1 Introduction

The purpose of this section is to present an outline of the procedures to follow in order to accomplish a few of the tasks which commonly face those engaged in groundwater data processing and modelling. The tasks are arranged in no particular order; nor is the list of tasks complete. It is intended that only a brief overview be presented of some of the possibilities afforded through use of the Groundwater Data Utilities. For details of the use of any particular program, see Part B of this manual.

4.2 Preparing Water Level Contours

To generate a contour map of water levels on or about a certain date, program SMP2INFO should be used to interpolate the water level data contained within a bore sample file to the date for which the contour map is desired. SMP2INFO generates a bore information file in which bore coordinates are included. This file can be presented to SURFER as an *xyz* data file for gridding and subsequent contouring.

The bore information file generated by SMP2INFO can also be used to post and label the bore locations on the contour map. Labels can consist of bore identifiers, or of borehole water levels interpolated to the user-specified date.

It is often desirable to include map data as a background to such a contour map. Most mapping and contouring programs require such graphical data in DXF format. If DXF mapfiles for the study area are unavailable they can be produced by digitizing roads, property boundaries, and watercourses from a map of the area using QDIGIT and converting the resulting line file(s) to DXF format using program QDIG2DXF. If DXF data pertinent to different geographical feature types are supplied to SURFER in separate files, the different feature types can then be displayed in different colours if desired.

To enhance the quality of the contour map, the grid file produced by SURFER at the data interpolation stage should be blanked at the aquifer boundaries (if they are clearly defined) or along a user-specified demarcation line where it is judged that contour lines are too distant from the nearest bores to be believable. There are a number of ways in which an appropriate SURFER blanking file can be constructed for this purpose. One way is to use the SURFER “Digitize” facility to construct a blanking file by digitizing directly from the screen. Another way is to construct a blanking file by slight modification of a QDIGIT line file based on digitized map data; however a user should be aware that a QDIGIT line file may possess a huge redundancy of data points for the reasons outlined in Section 3.4.

A third method is to construct a blanking file based on the boundary of the active part of a MODFLOW model grid. Firstly an integer array should be constructed in which all active and fixed head cells are assigned the same non-zero value, and all inactive

cells are assigned a value of zero (this can easily be accomplished through slight modification of a model activity array using the array editing capabilities of many MODFLOW graphical user interfaces). Then program ZONE2BLN can be used to construct a blanking file that will effectively blank any part of the SURFER grid that lies within the inactive part of the finite difference grid, or outside of the finite-difference grid altogether. As the active part of a finite-difference grid normally coincides with the aquifer, a blanking file produced in this manner blanks all contours where the latter are drawn outside of the aquifer.

It should be noted that a bore sample file can contain any type of borehole data, not just water level data. Hence contour maps of other time-variant aquifer characteristics such as chemical concentration can be produced in an identical manner to that described above for the production of water level contours.

4.3 Preparing Bore Hydrographs

In addition to providing a basis for the construction of aquifer iso-characteristic maps in the manner described above, water level or water quality data housed within a bore sample file can be extracted and plotted against time. Program SMP2HYD provides the functionality necessary to extract data for user-specified bores from a bore sample file, and to format it in a manner suitable for use by plotting packages such as GRAPHER, EXCEL, etc.

SMP2HYD can extract data for one or many bores. It can extract all of the historical data pertaining to a given bore, or can simply extract data between two specified dates and/or times. SMP2HYD's output files list borehole sample data together with time elapsed from a reference date and time; thus the data is in a form ready for immediate plotting. The units of elapsed time are user-selectable, as are the time and date of the temporal reference.

Using the functionality available through most commercial plotting packages, borehole data extracted by SMP2HYD can be plotted to any scale; multiple hydrographs can be placed on the same graph for easy comparison between bores if desired. For most packages the time axis can be annotated with either elapsed time or with actual dates and/or times.

4.4 Extracting and Manipulating Borehole Pumping Data

The amount of water pumped from user-specified bores between two-user specified dates can be calculated using program PMP2INFO. PMP2INFO obtains its data from a bore pumping file of the type illustrated in Example 2.5. The dates and times which define the beginning and end of a particular time interval need not coincide with borehole measurement times, for PMP2INFO interpolates between the latter times to the user-specified time interval endpoints. Pumped water units in the PMP2INFO output file are the same as those used by the bore pumping file.

The bore information file written by PMP2INFO tabulating borehole extracted volumes includes the geographical coordinates of each extraction (or injection) bore. Hence the PMP2INFO output file can be used by mapping software for posting pumping information on a map. For example a symbol can be placed on the map at each bore location, the size of the symbol being a function of the amount of water pumped.

PMP2INFO output files can also be used for transferring pumping data to a model, as discussed in the next section.

4.5 Importing Borehole Pumping Data into a Model

The assimilation of borehole pumping data into a model is one of the most time-consuming tasks in model preparation, especially for a transient model where such data must be supplied for each stress period. In irrigation areas where pumped bores may number in the hundreds, software support for this task is essential.

When using the Groundwater Data Utilities, the incorporation of borehole pumping data into a model is a two-stage process. First a bore information file must be produced for each stress period using PMP2INFO in the manner described in the previous section. For each stress period the appropriate bore information file will list the amount of water pumped during that period expressed in units used by the bore pumping file from which the data was extracted. Note that before this first processing stage can be implemented, a user must be aware of the date and time of the beginning and end of each model stress period.

The second step involves the assignment of borehole extraction rates to individual model cells. For MODFLOW modelling, borehole extraction can be supplied either through the well package or, if all extraction is from the same layer, as equivalent negative recharge through the recharge package. In either case, data can be transferred from a bore information file to the model using program PT2ARRAY.

PT2ARRAY reads a bore information file and a bore coordinates file. On the basis of the information contained in the former file and the coordinates contained in the latter file, it assigns values to those elements of a MODFLOW-compatible real array for which respective grid cells contain one or more bores. The values assigned to these elements can be modified by a scaling factor to take account of units conversion. A MODFLOW graphical user interface can then read the real array either as a recharge array, or, for some preprocessors, as a “well array”.

4.6 A Rudimentary Model-GIS Interface

There are a number programs within the Groundwater Data Utilities which provide a mechanism for integer and real array data exchange between MODFLOW/MT3D and a GIS. Real and integer arrays play a pivotal role in the parameterization and calibration of MODFLOW, MT3D and other finite-difference models such as SHARP. Their importance in data exchange between models, GIS, model

preprocessors and visualisation software is further enhanced by the fact that most MODFLOW graphical user interfaces provide the ability to import and export MODFLOW/MT3D data arrays.

Programs INT2MIF and REAL2MIF each produce files in MAPINFO Interchange Format, the former based on a MODFLOW/MT3D-compatible integer array, the latter based on a MODFLOW/MT3D-compatible real array. The “MIF” file supplies MAPINFO with the geographical information which it needs in order to plot the finite difference grid (or a subset of the finite difference grid defined by a “window” integer array) on a map; the respective “MID” file contains a table listing the value of each element of the integer or real array, each element being identified by its row and column number. This table can be edited within MAPINFO, either on a cell-by-cell basis, or using GIS functionality based on the properties of other geographical layers covering the same area. The edited table can then be downloaded, converted to integer or real array format using program TAB2INT or TAB2REAL, and imported into a model graphical user interface, or used by MODFLOW or MT3D (or any other cell-centered finite difference model such as SHARP) directly.

A rudimentary model-ARCINFO interface mechanism is provided through program GRID2ARC. GRID2ARC writes a file in ARCINFO “generate” format containing the geographical information pertaining to a subset of the finite difference grid, the subset being defined by a “window” integer array.

4.7 Making Pictures of the Model Grid

Most graphical model preprocessors allow a user to export pictures of a model grid in DXF format. However in many cases the ability to export only a subset of the grid (for example active cells only) is limited. Also, while it is often possible to obtain pictures of grid zonation in which zones of constant integer or real array value are represented in different colours, it is rarely possible to obtain a DXF file containing grid zonation boundaries represented as polylines, thus providing the basis for a more appropriate means of schematizing grid zonation on black-and-white printers and photocopiers.

Programs GRID2DXF and ZONE2DXF produce DXF files of a subset of the finite difference grid, and of the outlines of multi-cell zones within the finite difference grid respectively. The latter are defined in terms of groups of cells of constant value contained within a MODFLOW /MT3D-compatible integer array. The resultant DXF files can be imported into most mapping software where lines can be coloured and thickened as desired. A pleasing effect can be obtained by drawing the active part of the finite-difference grid using fine lines and superimposing internal grid zonation boundaries using heavier lines. Another useful context for the plotting of grid zonation boundaries is in the reporting of grid zonation values; the latter can be written as text within the grid zonation schematic.

Functionality also exists within the Groundwater Data Utilities for generating SURFER “blanking” files of the finite difference grid and of the zonation contained

within this grid in a manner analogous to the production of DXF files of these same features. Programs GRID2BLN and ZONE2BLN are identical to GRID2DXF and ZONE2DXF except that they generate blanking files instead of a DXF files. Pre-WINDOWS versions of SURFER, which were unable to read DXF files, imported line data as blanking files. While the newer versions of SURFER are still capable of using blanking files in this manner, the principal use of this type of file is in blanking parts of the SURFER grid so that contour lines are not displayed in areas where they are not relevant. As was discussed in Section 4.2, a blanking file produced by ZONE2BLN can be very useful in restricting contour lines to within aquifer boundaries.

4.8 Interpolating Model-Generated Heads to Boresites

The data contained within MODFLOW and MT3D-generated unformatted head, drawdown, concentration and other two-dimensional arrays can be interpolated to the sites of bores using program MODBORE (or MT3BORE) from the PEST MODFLOW/MT3D Utilities suite. See Doherty (1995) for further details. As is explained in that manual, it is important when undertaking model calibration that model-generated contours are constructed in exactly the same way as are field contours. This involves interpolating model-generated water levels or concentrations to the same data points as those from which measured water levels or concentrations were taken, and then contouring this interpolated data using exactly the same contouring options as were used for contouring the field data.

Another mechanism for comparing field and model-generated data is through the use of program MOD2SMP from the Groundwater Data Utilities. MOD2SMP constructs a bore sample file from a set of MODFLOW/MT3D-generated head, drawdown, concentration or other two-dimensional arrays (these are written in unformatted form during each model run). During construction of the bore sample file the model results arrays are interpolated to a set of user-specified points, these points usually being the sites of bores from which field measurements were taken. Sample dates and times written to the bore sample file correspond to model output times; the user is asked for a reference date and time corresponding to the beginning of the model run.

Once a bore sample file has been constructed on the basis of model-generated data interpolated to boresites, comparison of field and model data is a simple task. In particular, program SMP2INFO can be used to construct contour maps of field and model data for any user-specified date. Program SMP2HYD can be used in the construction of bore hydrographs for both model and field data. Using software such as GRAPHER, model and field hydrographs for one or a number of bores can be superimposed for ease of comparison.

4.9 Constructing a Section through a Model

Using program SECTION a transect of arbitrary complexity can be constructed through the model domain. SECTION produces files that can be plotted by software

such as GRAPHER and EXCEL; its role is to extract and interpolate model data upon which the plot is to be based.

SECTION uses a similar spatial interpolation algorithm to MODBORE and MOD2SMP; it interpolates data contained in MODFLOW/MT3D-compatible real arrays to a regular set of points of user-defined density along a transect line with user-defined endpoints. It can assimilate data from one or many arrays. Thus if it is supplied with a land surface elevation array, aquifer top and bottom elevation arrays and a model-generated heads array, the file written by SECTION can be used to generate a picture of the aquifer showing its top and bottom, as well as the land surface and the piezometric surface, the latter generated by the model. By incorporating the top and bottom elevations of other layers and/or model-generated heads at other model output times, a complex, yet instructive, picture of subsurface conditions can be constructed.

4.10 Using SURFER to Construct an Initial Conditions Array

A number of MODFLOW/MT3D pre- and postprocessors include the functionality whereby aquifer data obtained on a point-by-point basis can be spatially interpolated to the finite difference grid in order to produce initial condition arrays. However interpolation options are often limited so that the array of initial conditions is often far from satisfactory. This is of particular concern in the case of initial heads arrays; a model may spend the first few time steps of its simulation in simply moving water between cells as rapidly as possible in order to compensate for an initial heads array that has unnecessary “bumps”, or that causes water to temporarily flow in unusual directions simply as an artefact of the interpolation scheme used in its construction.

If a model finite difference grid is uniform, SURFER can be used to interpolate point data to the finite-difference grid cell centres. SURFER possesses many more interpolation options than do most model preprocessing packages, including the “minimum curvature” method which (in the author’s experience) often results in an array that functions well as an initial conditions array. If a SURFER grid is constructed such that x and y direction grid lines intersect at finite-difference grid cell centres, then the contents of a SURFER grid file can be used directly as a model real array. However the grid file (which must be stored in ASCII form) must first be translated into model-compatible real array format before importation into a MODFLOW preprocessor; this can be accomplished using program SRF2REAL.

A problem occurs where the grid is uniform but is not oriented with its row direction east-west and its column direction north-south, for a SURFER grid can only be thus oriented. In this case the model grid must be rotated so that it can be simulated by a SURFER grid. However not only must the model grid be rotated, but the data used to construct the initial conditions array must also be rotated. Program ROTDAT carries out the latter function, transforming point coordinates data contained in an xyz file in a manner equivalent to rotating all data points about the top left corner of the finite difference grid, and assigning the latter point x and y coordinates of (0,0). If the rotated and translated data is then read by SURFER and interpolated onto a grid

which is equivalent to the finite difference grid in terms of its number of rows and columns, but for which the top left intersection point (ie. node) is situated at $(delr/2.0, -delc/2.0)$, the grid file thus produced can be translated into a real array file by SRF2REAL for immediate model use. Here *delr* is the (uniform) model cell width in the row direction while *delc* is the (uniform) model cell width in the column direction.

Note that if a grid is nonuniform, SURFER can still be used in the production of initial conditions arrays, though now a two-step process is required. The first step is to grid the point data using SURFER to a fine grid which is large enough to cover the entire model area (no grid rotation or translation is required). The SURFER grid can then be stored as an *xyz* file to be subsequently used by a model preprocessor's interpolator for the production of a model initial conditions array. The fact that the second stage interpolator may not be very good is of little consequence because *xyz* data points are close to all model cell centres, thanks to first stage interpolation to a dense grid carried out by SURFER.

4.11 Using SURFER to Display Model Results

Section 4.8 discusses the means whereby model results can be interpolated to boresites for subsequent display as either individual hydrographs or as contours. However if a model grid is uniform, a model-generated real array can be translated into a SURFER grid file using program REAL2SRF. This grid file can be directly read by SURFER as if it had constructed it itself; thus no intermediate interpolation is required and SURFER is able to construct contours on the basis of "raw" model data.

If the uniform model grid is oriented with its row direction east-west and its column direction north-south, map data can be directly overlain on the contour map generated by SURFER on the basis of the grid file built by REAL2SRF. However if the grid row direction is oriented at an angle other than east-west, REAL2SRF writes the SURFER grid file using coordinates that effectively rotate and translate the grid until the row direction is oriented east-west and the top left corner of the grid is at the point (0,0); this rotation and translation operation is necessary because a SURFER grid can only be oriented with its *x* direction pointing east and its *y* direction point north. Any map data that is to be overlain on a contour map built from this grid file must likewise be rotated and translated. The functionality to undertake this data rotation and translation is available within the Groundwater Data Utilities. The contents of a DXF file can be appropriately transformed using program ROTDXF. Program ROTBLN transforms the contents of a SURFER blanking file. *xyz* data can be transformed prior to posting on the SURFER-generated contour map using program ROTDAT.

Once SURFER has produced its contour map, and map data (transformed as above) has been overlain on it, the composite picture should then be rotated to its true orientation using the SURFER "Arrange/Rotate" menu item. Note, however, that axis labels will still reflect the artificial, rotated and translated coordinate system, and should thus be eliminated from the plot.

If a model finite difference grid is not uniform the above method cannot be used to export model results to SURFER. In this case, if it is desired that SURFER be used to display model results, SURFER should be presented with an *xyz* file containing the model-calculated head (or concentration, etc.) at each active cell centre. SURFER can then grid this data using one of its internal gridding algorithms prior to displaying the results. The interpolation method will not matter too much as no SURFER grid point will be too far from a model-specific *xyz* point (except where the SURFER grid over-reaches the active part of the model grid; in this case over-reaching segments should be blanked using one of the methods described in Section 4.2 above).

The construction of an *xyz* file of model results at all active cell centres is a two-step process. First a file tabulating the coordinates of active cell centres must be constructed; next model results must be interpolated to these points. The first step can be accomplished using program GRID2PT; the second can be accomplished using program MODBORE from the PEST MODFLOW/MT3D Utilities suite, or by using program MOD2SMP followed by SMP2INFO, these latter two programs belonging to the Groundwater Data Utilities. Note that the latter method could involve the production of very large files if the number of active cell centres is large. However the length of this file could be minimized by limiting model-generated unformatted output to the time step of interest.

4.12 Extracting Model-Generated Arrays

MODFLOW and MT3D generate unformatted data files containing two-dimensional arrays of head, drawdown, concentration, etc data. These files cannot be inspected with a text editor as data are represented in binary format.

Program MANY2ONE has been designed to extract individual arrays from MODFLOW and MT3D unformatted output files and re-write them in formatted form where they can be viewed with a text editor and/or transferred to model pre- and postprocessing packages. Because MANY2ONE displays the header to each array as it peruses a MODFLOW or MT3D unformatted data file, it can be used to explore the contents of such a file; the header lists the data type, model stress period, time step (and transport step) to which each array pertains. As each header is displayed, MANY2ONE provides a user with the option of extracting that array or of moving on to the next array.

4.13 Array Data Manipulation

Mention has already been made within this report of the importance of integer and real arrays in MODFLOW/MT3D pre- and postprocessing. The ability to transport such arrays between MODFLOW Graphical User Interfaces and the Groundwater Data Utilities, visualisation and mapping software such as SURFER and GIS, and the model itself is fundamental to flexible and powerful model data processing and results analysis. Because of the importance of model data arrays in the overall modelling effort, a number of Groundwater Data Utilities carry out various types of array processing and manipulation.

Program INT2REAL builds or modifies a real array based on the contents of an integer array. This is especially useful where an integer array defines spatial parameter zonation. For example an integer array may define land use units throughout a modelled catchment. The effects of different land use strategies on groundwater levels may be tested by building different recharge arrays on the basis of the integer array, recharge rates being assigned on the basis of the land usage pertaining to each zone. Using INT2REAL real arrays can be built from scratch, or an existing real array can be modified within user-specified zones.

Program REAL2INT builds an integer array from a real array either on the basis of a one-to-one correspondence between real and integer array elements, or by assigning integer array values on the basis of value ranges within the real array. The integer array can then be used in further processing or for display. For example, through the use of ZONE2DXF a black-and-white picture of array zonation boundaries can be superimposed on a background map plotted using most mapping software.

Program TWOARRAY carries out mathematical operations (including partial array replacement) between two MODFLOW/MT3D compatible real arrays. All operations are such that user-specified portions of an array can remain unaffected by the manipulations.

The role of MANY2ONE in selecting individual results arrays from a MODFLOW or MT3D output file has already been discussed in Section 4.12 above.

4.14 PEST and the Groundwater Data Utilities

The present section discusses a number of ways in which programs of the Groundwater Data Utilities can be used in conjunction with PEST to add enormous flexibility and power to the model calibration process. However you should also read Section 5 of this document where the use of pilot-point-based parameterisation is discussed. As is described in that section, it is possible, using programs from the Groundwater Data Utilities, to instigate a model calibration process based on the use of pilot points, complemented by the imposition of geostatistically-based constraints on parameter values using PEST-ASP's powerful regularisation functionality. The power that this brings to the calibration process is awesome!

The Groundwater Data Utilities can be used in conjunction with PEST and its utilities to construct an extremely powerful modelling system. The fact that the Groundwater Data Utilities are executed from the command line allows them to be run from within a batch file as part of a “composite model”. This composite model can be run by PEST in order to calibrate it against field data of various types.

In most cases such a composite model will include MODFLOW and/or MT3D. Some of the Groundwater Data Utilities can be run from within the batch file as preprocessors to one or both of these models; others can be used as postprocessors. Others can be run outside of the batch file for automatic PEST input file generation.

A MODFLOW-compatible real array can be constructed on the basis of a MODFLOW-compatible integer array using program INT2REAL, the integer array being used to define zonation for a particular model layer; the real array can then be “pasted” into an existing MODFLOW input file using program REPARRAY. Integer-real correspondences can be stored within an “integer-real correspondence file”. A PEST template file is easily built from such an integer-real correspondence file. This represents an efficient mechanism for estimating parameters pertaining to certain model domain zones, for it is far easier to construct a template file based on an integer-real correspondence file than to build a template file based on a MODFLOW input file (especially where elements occurring within large arrays are in need of estimation). The first part of the composite model will then be comprised of INT2REAL, followed by REPARRAY, followed by MODFLOW. In all cases the answers to command-line prompts generated by these programs should be written to a file using a text editor, and supplied to the program using command line redirection. A program such as INT2REAL is thus run from within the batch file using a command such as:-

```
int2real < int2real.in
```

where file `int2real.in` contains pre-recorded answers to INT2REAL’s prompts.

Complex real array manipulation can be undertaken between generation of one or more real arrays on the basis of one or more integer arrays, and the pasting of one or more arrays into an existing MODFLOW dataset. Such array manipulation can be carried out with program TWOARRAY which must thus be executed from within the composite model encapsulated in the model batch file.

Once MODFLOW or MT3D has been run, model-generated water levels or solute concentrations will often need to be spatially interpolated to the sites of boreholes. This can be accomplished using program MOD2SMP, the outcome of MOD2SMP’s execution being a bore sample file. This operation allows field data to be compared with model data. For a more exact comparison, model-generated heads and solute concentrations can also be *temporally* interpolated to the *times* at which measurements were taken, in addition to being *spatially* interpolated to the *locations* of field measurements. This dual time-space interpolation can be carried out using program MOD2OBS; the outcome is, once again, a bore sample file. If this is done, MOD2OBS must be called from within the composite model batch file after MODFLOW and/or MT3D have been run from within this same file.

Inflows and outflows of water to/from the model domain within each of a number of user-specified zones can be tracked from time step to time step using program BUD2SMP. The outcome of this operation is, once again, a bore sample file. Using BUD2SMP inflows and outflows are recorded at times for which such information is generated by MODFLOW. If program SMP2SMP is run after BUD2SMP, another bore sample file is generated in which model inflow/outflows are *temporally* interpolated to the *times* at which field measurements are recorded in another bore sample file. Thus a direct comparison can be made between field measurements and model outputs.

If either MOD2OBS or SMP2SMP is used to build a model-generated equivalent to an existing measurement-based bore sample file, model results and field measurements can be directly compared on a one-to-one basis. Through the use of program PESTPREP, a suite of PEST input files can then be generated through which a PEST run can be undertaken in order to adjust specified model parameters until the discrepancies between model and field data are reduced to a minimum in the weighted least squares sense. Through the use of PESTPREP preparation for a PEST run can be reduced to minutes, even where observation datasets are very lengthy. The model that is actually run by PEST is thus a batch file comprised of MODFLOW and/or MT3D together with MOD2OBS, or BUD2SMP followed by SMP2SMP (or even all three of these postprocessors), possibly in conjunction with one or a number of preprocessors as described above.

The ability to build a composite model according to the demands of a particular modelling application, and to obtain model outputs which are both spatially and temporally interpolated to the places and times of field measurements, complemented by the ability to automate generation of PEST input files for systems of arbitrary complexity, constitutes an extremely powerful modelling system.

4.15 Model Inflows and Outflows

Although programs such as ZONEBUDGET allow a user to obtain model-calculated water exchange rates between various user-specified zones within a model domain, the output files generated by this and other, similar, programs are not normally in a form whereby the variation of this inflow or outflow over time can be easily plotted. Such functionality is available, however, through program BUD2HYD. If cell-by-cell flow terms are recorded during a transient MODFLOW run, BUD2HYD is able to extract flow rate data generated by user-specified packages throughout the simulation time, and to format this data in a manner readily acceptable by most commercial plotting packages. This makes it easy to generate graphs of, for example, river baseflow or mine inflow against time through a model simulation period.

5. Model Parameterisation based on Pilot Points

Note: since the time of writing this section I have written a number of new programs which provide assistance in pilot point and stochastic parameterisation of a groundwater model. These are FIELDGEN, ARRAYOBS, REAL2TAB and VERTREG. See Part B of this manual for a description of the individual programs. I'll add some details to this section when I have the time.

5.1 Introduction

A number of programs supplied with the Groundwater Data Utilities can be used to assist in spatial property definition across a model domain. In doing this they can replace, or at least complement, spatial parameter definition based on zonation. When employing zones to define the distribution of some hydraulic property over a model domain, that property is assumed to be uniform within each such zone. Although zone boundaries are often defined in such a way as to coincide with mapped geological boundaries, zonation as a means of parameter definition is often unsatisfactory for at least the following reasons:

- the locations of geological boundaries are often subject to a large degree of uncertainty, especially in areas where outcrop is scarce;
- the disposition of geological units with depth is often poorly known;
- rock types that are grouped into similar geological units for the purposes of producing a map may have very different hydraulic properties, and thus may not constitute a proper grouping from a hydrogeological point of view;
- even where geological grouping is based on perceived hydraulic similarity, hydraulic homogeneity can rarely be guaranteed.

The last of the above points is of particular importance. It is rare that a zonation based on geological characterisation does not need some refinement as the model calibration process (which can be considered as a form of data interpretation) exposes the fact that heterogeneity, in addition to that encompassed in the current zonation pattern, must prevail within the model area if model outputs are to match field observations to an acceptable degree. The problem then arises as to how much additional zonation should be introduced to the model domain, and where the boundaries of new zones should be drawn. Furthermore, once enough zones have been introduced to the model domain to allow a good fit between model outputs and field data to be achieved, the resulting zonation pattern can look artificial. Justification for the introduction of extra zones is based on the fact that the calibration process has proved that heterogeneity exists, and to thus ignore this heterogeneity would be worse than adopting a zonation pattern which is somewhat arbitrary and which, due to the fundamental nonuniqueness of the calibration problem, is probably one scheme amongst many

others that would also have provided an acceptable fit between model outputs and field data.

The present section describes an alternative method of model domain parameterisation based on geostatistics and pilot points. It does not, by any means, remove the fundamental nonuniqueness of the parameter estimation problem. However the main advantage of the method is that it allows parameter definition to take place in a more flexible manner than through the use of zones. This, in turn, allows more powerful methods of model parameter estimation to be applied to the model calibration problem, particularly those which are made available through the use of PEST's predictive analysis and regularisation capabilities.

When used in regularisation mode in conjunction with a parameterisation scheme that allows smaller scale hydraulic property variations to be represented than can be specified on the basis of zones alone, PEST can be asked to make a model domain (or individual zones within a model domain) only as heterogeneous as it needs to be in order to achieve an acceptable level of fit between model outputs and corresponding field data. "Regularisation constraints" necessary to achieve this "minimum heterogeneity" condition can be designed in such a way as to reflect any available geostatistical or intuitive evidence within a study area pertaining to any heterogeneity that might exist. Such evidence normally takes the form of a specification that hydraulic property differences between two points are likely to be smaller if the two points are closer together than if they are further apart. Furthermore, the capacity of the parameterisation scheme to allow small scale heterogeneity to be represented allows PEST to place such heterogeneity only at those locations where it will "do the most good" from the point of view of matching model outputs to field data.

Use of PEST in predictive analysis mode is similar to its use in regularisation mode in that parameterisation of the model domain (or of zones within the model domain) is also "conditioned" by imposition of an external constraint. In predictive analysis mode, this constraint is the maximisation or minimisation of a particular model prediction. Flexibility in spatial parameter definition achieved through the use of pilot points allows PEST to ascertain the full range of uncertainty pertaining to a particular prediction where this range is dependent on the existence or otherwise of geological heterogeneity (as it often is, particularly in the case of solute transport).

5.2 Geostatistical Concepts

The purpose of this section is to provide the geostatistical underpinnings of the pilot-point-based parameterisation methodology implemented through a number of the Groundwater Data Utility programs documented in Part B of this manual. Only limited information is provided on geostatistical methods in general. Many excellent texts on that subject are now available. See, for example, Deutsch and Journel (1998) - a description of the GSLIB library upon which the software described herein is based.

Where pilot points are used as the basis for hydraulic property definition throughout a model domain, values of that property are first defined at the locations of the points. Hydraulic property values are then assigned to all cells within the model domain through spatial interpolation of the values assigned to the pilot points. As presently implemented, such spatial interpolation takes place using the method of kriging. As is described in any geostatistical text, this method is intended to minimise the uncertainty of the property estimate at each interpolated point, based on an assessment of the spatial variability of that property as specified by a variogram. Use of a variogram to characterise spatial heterogeneity is based on the premise that the closer are two points situated with respect to each other, the more likely are their properties to be similar, and that the degree to which this premise holds true does not vary across a study area or geological unit.

Four types of variogram are supported by programs of the Groundwater Data Utilities that implement the pilot-point-based parameterisation scheme described herein. They are as follows:-

Spherical

$$\gamma(h) = c \cdot \left[1.5 \frac{h}{a} - 0.5 \left(\frac{h}{a} \right)^3 \right] \quad \text{if } h < a \quad (5.1a)$$

$$\gamma(h) = c \quad \text{if } h \geq a \quad (5.1b)$$

Exponential

$$\gamma(h) = c \cdot \left[1 - \exp\left(-\frac{h}{a}\right) \right] \quad (5.2)$$

Gaussian

$$\gamma(h) = c \cdot \left[1 - \exp\left(-\frac{h^2}{a^2}\right) \right] \quad (5.3)$$

Power

$$\gamma(h) = c \cdot h^a \quad (5.4)$$

where the variogram, $\gamma(h)$, is defined by the equation:-

$$2\gamma(h) = E\{[Z(x) - Z(x + h)]^2\} \quad (5.5a)$$

Here $Z(x)$ is the value of a certain hydraulic property at location x , and h is the separation between two points at which the property is measured or defined. (“ E ” stands for “expected value”.)

It is easily shown that $2\gamma(h)$ is thus equivalent to the variance of the difference between hydraulic property values pertaining to points a distance h apart taken over the area where the variogram is applicable; ie.

$$2\gamma(h) = \text{Var}[Z(x) - Z(x + h)] \quad (5.5b)$$

Variograms can be applied to native hydraulic properties, or to transformed property values (most often log-transformed property values). Furthermore, a variogram can be isotropic or anisotropic. In the latter case specification of the variogram requires that the direction of elongation of the ellipse of anisotropy be supplied. For the utilities described herein this can be oriented at an arbitrary angle to the finite difference grid.

Variograms can be “nested” to form a “geostatistical structure”; for the programs described herein, full characterisation of the geostatistical structure of an area can be based on the summation of up to 5 separate variograms plus a “nugget” (ie. a fully random component with no spatial correlation). Individual variograms within a nested structure can be of different types and of different anisotropy. In the groundwater context, however, it is rare that spatial variability will be characterised in enough detail to require more than one variogram for its specification.

Two types of kriging are permitted in the programs described herein, viz. “simple kriging” and “ordinary kriging”. The difference between these is discussed in any geostatistical textbook. In general, it is better to employ ordinary kriging when using pilot points to parameterise a model domain (this is the most commonly applied method of kriging anyway), for simple kriging requires that the mean value of the hydraulic property throughout the model domain be specified. For reasons that are explained below, this creates certain inefficiencies in the parameterisation process, especially when using nonlinear parameter estimation techniques for model calibration.

One of the advantages of using kriging as a method of spatial interpolation is that the factors by which property values at known points (ie. pilot points) are multiplied to obtain property values at unknown points are independent of the property values at the known points. Thus a set of “interpolation factors” can be calculated in advance, and re-applied to the property values assigned to pilot points as these values are updated. This makes the method ideal for use in the nonlinear parameter estimation context where property values at pilot points are continually updated as the parameter estimation process proceeds.

Another benefit of using kriging for spatial interpolation is that kriging is an “exact interpolator”. This means that the interpolated property value at the location of each pilot point is equal to the property value assigned to that pilot point.

As a by-product of spatial interpolation using kriging, the uncertainty of interpolated property values can be calculated together with the interpolated property values themselves. This uncertainty estimate, too, is independent of the hydraulic property values assigned to the pilot points. Because this uncertainty can be calculated at all points throughout a model domain at which spatial interpolation is required (normally the centres of finite-difference cells), it can be visualised using the contouring and/or shading functionality available through a model array editor/viewer. Note, however, that calculation of uncertainty in this manner assumes minimal uncertainty associated with property values at pilot points. Where the latter are estimated as part of the model calibration process, this is certainly not the case. However such a contour map may be useful in judging where to add more pilot points if it is felt that extra points are warranted.

5.3 Parameter Estimation Using Pilot Points

When parameterisation of a model domain is based on pilot points, PEST can be used to estimate the hydraulic property value pertaining to each of the pilot points. These values are then spatially interpolated to the centres of pertinent active cells within the model domain using kriging based on one or more of the variograms discussed above. Thus in assigning values to pilot points, PEST is actually implicitly assigning hydraulic property values to part or all of the model domain.

There is no fundamental reason why kriging should be used for spatial interpolation between pilot point values rather than another method of spatial interpolation, for example inverse-power-of-distance, multiquadratic, splines, linear interpolation based on triangulation, etc. However there are some advantages to the kriging method that make it attractive for use in this role. Some of these have already been mentioned. Another one is that kriging tends to produce rather smooth, regular, interpolated property fields whereas some methods, such as splines, can produce “wavy” surfaces, especially if two pilot points are close together and are assigned very different property values. However, in this regard, kriging based on some variograms is better than kriging based on others. Experience has demonstrated that kriging based on the Gaussian variogram sometimes leads to spurious interpolated property fields. In general, kriging based on the exponential variogram seems to be the best behaved. Furthermore, it is often better to interpolate the logarithms of hydraulic properties assigned to pilot points rather than native hydraulic property values, for the resulting hydraulic property fields are often more regular and have a more realistic appearance. In fact the groundwater literature cites many examples where the hydraulic conductivity or transmissivity distribution within a study area is better characterised by a log variogram than a native variogram.

In spite of its advantages, care must always be taken when using kriging as a spatial interpolator. In some instances kriging factors can be negative, especially if using the

Gaussian variogram. This can lead to interpolated properties which are greater than the highest property value assigned to any pilot point, or lower than the lowest property value assigned to any pilot point. Sometimes this can lead to spurious interpolated property values over parts of the model domain. To mitigate the adverse effects of such over- or under-estimation, the kriging utilities described herein allow the user to set maximum and minimum interpolated property values. A single value for each of these can be supplied, applicable to the entirety of the model domain, or maximum and minimum interpolation limits can be supplied on a cell-by-cell basis.

5.4 Variogram Selection

There are very few cases of groundwater model deployment where enough hydraulic properties have been measured at enough points to determine variograms which accurately describe the spatial distribution of these properties. In most cases this does not really matter, for in the present context variograms such as those described in Section 5.2 are more useful as an interpolation device than as an accurate representation of hydraulic property heterogeneity within a model domain. Furthermore, if hydraulic property values at pilot points are estimated as part of the model calibration process, it is not possible to determine a variogram in advance based on property values pertaining to these pilot points.

If kriging is based on a single variogram, rather than a nested variogram structure, the value of c in each of equations 5.1 to 5.4 does not affect hydraulic property values calculated through spatial interpolation of pilot point values (unless it is set too high when using the power variogram). However it does affect the kriging variance associated with interpolated values. Fortunately this is of little concern in the present context.

A little care must be taken in selection of an appropriate value for the parameter a in each of equations 5.1 to 5.4. In the first three of these equations a is related to the “range” of the variogram, this being the distance at which the variogram has almost reached its maximum value. In general, depending on the geometry of a study area and the number of pilot points used in the parameterisation process, a range of between one fifth and two thirds of the size of the model domain (or of a zone within the model domain in which these pilot points are situated) is suitable in most cases. The reason for this is more practical than scientific. If the range is shorter than the distance between most pilot points, then interpolated property values over much of the model domain will tend towards the average value of all points within the domain (or at least of those points within the search radius used for selection of points for interpolation to any particular cell centre). When pilot points are used in conjunction with PEST for flexible characterisation of spatial property distribution, this will hamper PEST’s ability to impose any kind of hydraulic property “structure” over the model domain such as might be required if the model is to produce outputs which match field data well.

For the spherical variogram listed in Section 5.2 the range is approximately equal to a . for the exponential and Gaussian variograms the range is approximately equal to

3a. The power variogram has no range, for there is no distance at which the variogram reaches an upper limit. In this case the value for the variable a should be selected in such a manner that application of equation 5.4 yields a realistic estimate of the expected degree of spatial variability of a particular hydraulic property (or of its logarithm) over the model domain.

The value selected for anisotropy of a variogram can be critical in determining the nature of a spatially interpolated hydraulic property field. Anisotropy is generally defined as the ratio of the variogram range in the direction of maximum spatial uniformity to that in the direction of minimum spatial uniformity; thus it is generally greater than or equal to 1. As well as the magnitude of the anisotropy, the bearing of the direction of greatest uniformity must also be supplied as part of the geostatistical characterisation of an area on which kriging interpolation is based.

It should be noted that in using the utilities described herein, different variograms (with different properties) can be assigned to different zones within the model domain; thus these different zones can represent geological units with very different geostatistical structures.

It is not unreasonable to ask why the variables governing the shape of a variogram cannot be estimated together with the pilot point properties themselves as part of the nonlinear parameter estimation process. In theory, there is no reason why this cannot be done. However, in some instances there are definite disadvantages associated with this approach. The first is that, once the range has reached a certain value, model outputs tend to be insensitive to it (and, of course, if a geostatistical structure contains only one “nested” variogram they are completely insensitive to c). The second is that if the range is estimated at the same time as the pilot point property values, then kriging weights must be continually re-calculated. This can be a very time-consuming process and can lengthen the time required for a PEST run considerably. However if the properties of the variogram remain invariant, then the same set of kriging factors can be used for every model run. (Note however that use of PEST-ASP’s multiple command-line functionality has the potential to make simultaneous estimation of pilot point values and variogram properties a little more attractive.)

For similar reasons, ordinary kriging, rather than simple kriging, should be used on most occasions on which parameterisation of the model domain is effected through the use of pilot points. When simple kriging is used, kriging factors depend on the (externally-supplied) mean hydraulic property value over a model domain or zone. Thus if the mean is estimated as part of the calibration process (which will normally be the case) all kriging factors need to be updated as the parameter estimation process progresses. Once again, this can be a very time-consuming procedure.

Another advantage of using ordinary kriging rather than simple kriging in most instances of pilot point parameterisation is that, because the mean is not specified (or estimated) over a model domain or zone, it can effectively be allowed to vary spatially over this domain or zone by limiting the number of pilot points used in spatial interpolation to each cell centre on the basis of a “search radius”, or by simply specifying the maximum number of points to be used in any one calculation of an

interpolated value. The greater the search radius, the more homogeneous is a spatially interpolated property field likely to be. A smaller search radius can thus promote a greater degree of spatial variability; however it also limits the stability of the kriging process, and the effectiveness of any kriging-based regularisation employed in the parameter estimation process (see below).

In most cases where kriging is used in conjunction with pilot points for model parameterisation, a nugget value of zero should be used. However a non-zero nugget value can sometimes mitigate the effects of instability incurred through use of the Gaussian variogram. However, to be on the safe side, it is best to avoid the use of this type of variogram in the present context.

5.5 Locations of Pilot Points

When using pilot points for model parameterisation the user must decide where these pilot points should be placed. For some points the answer will be obvious; for example if hydraulic properties were measured in a bore (and if it is reasonable to assume that borehole-measured properties are suitable for use in a groundwater model), then a pilot point should be placed at the site of that bore. The property value assigned to that point may then be fixed during the parameter estimation process.

The locations of other pilot points may not be so easy to determine. However in most instances there are a number of simple criteria which can help in the selection of pilot point locations. One such criterion is that there should be a “good spread” of these points throughout the model domain or zone within which they are employed. This may necessitate that some points be placed at the boundaries of the model domain (often far removed from the sites of borehole head measurements or river flow measurements employed in the model calibration process); by placing some points near the boundaries, they can be used in conjunction with internal points to enforce some “structure” on the disposition of interpolated hydraulic properties throughout the model domain or zone; if such boundary points were absent, interpolated hydraulic property values may tend towards the mean of pilot point values as the boundary is approached, a situation that may prevent a good fit between model outputs and field observations from being achieved in certain hydraulic settings due to the constraints thus imposed on the hydraulic property interpolation process.

Another criterion that can be used to assist in the placement of pilot points is that they should not be placed too close together unless this is necessary for the model to obtain a good replication of disparate field measurements at nearby sites. As was mentioned above, if pilot points are placed too close together, instability of the kriging process can occur in some situations, particularly if using a Gaussian variogram. However, provided proper caution is exercised, it is often a good idea to place pilot points between bores in which there is a substantial head differential, in order that PEST can assign values to these points in a manner that is most beneficial for reproducing the head difference between these bores using the model.

Another guiding principal is that, if possible, pilot points should be placed at locations at which key model predictions are most sensitive to their values. This can be particularly useful when PEST is used in predictive analysis mode in order to infer the effects of unknown, but plausible, geological heterogeneity on these key model predictions.

5.6 Regularisation

One of the main advantages of using pilot points in preference to zones (or in combination with zones) is that the modeller does not need to define the “hydrogeological structure” of the model area ahead of the parameter estimation process. For example, in a certain study area it may be apparent from the shapes of piezometric contours, and from an inability to achieve a satisfactory fit between model outputs and borehole-measured heads based on a simple parameterisation of the model domain, that the subsurface is heterogeneous. However it may be very difficult to determine a zonation pattern that improves model-to-measurement fit to a desired level. In practice, a modeller will probably design a zonation pattern over the model domain based on intuition, geological insight, the shapes of piezometric contours and the results of previous calibration attempts, and will then use PEST to optimise the hydraulic properties assigned to these zones. If a satisfactory fit between model outcomes and field observations can be obtained for any particular zonation pattern, then this is taken as a necessary, but not sufficient, condition for acceptance of that zonation pattern. However, due to the inherent nonuniqueness of the inverse problem, there will almost certainly be other (possibly quite different) zonation patterns which will also do the job. But a modeller will rarely have the time, or the patience, to search for too many of these alternative patterns.

If a modeller is unsure of the hydrogeological structure prevailing within a certain area, an alternative calibration methodology is to “let PEST find the structure” by calibrating the model on the basis of a superfluity of pilot points scattered liberally throughout the model domain. Such parameter redundancy on its own will probably result in very poor PEST performance because, as is explained in the PEST manual, over-parameterisation leads to high parameter correlation, parameter insensitivity and a singular normal matrix. The result is normally a spectacular failure to lower the objective function much at all.

However if the superfluity of pilot points is combined with regularisation information, and if PEST is asked to optimise parameters while working in regularisation mode, then its performance in optimising these parameters can often be quite spectacular. Furthermore, because of the superfluity of pilot points scattered throughout the model domain, PEST is able to establish the hydrogeological structure itself through the way in which it assigns property values to these points in order to reduce the model-to-measurement misfit as much as possible. The problem of having to test different zonation patterns is thereby eliminated.

As is explained in the documentation to PEST-ASP, regularisation is the imposition of a set of relationships between parameters (or between functions of parameters),

added to the calibration process as either observations or prior information. The addition of these relationships often brings uniqueness to the parameter estimation problem, even where there are far more parameters requiring estimation than it would be possible to accommodate on the basis of the observation data alone. If regularisation conditions are properly defined, parameterisation uniqueness (and hence numerical stability) results from the fact that these conditions on their own would be sufficient, or nearly sufficient, to parameterise the model domain, even if there were no data. (Of course, the addition of data to the calibration process results in a very different set of parameters than would be calculated if there were no such data.)

When used in regularisation mode, just as in parameter estimation mode, PEST is asked to ensure that the fit between model outcomes and field observations is as good as possible. However it is asked to do this in such a way that the departure between calibrated parameter values and an “ideal” parameterisation (as suggested by the regularisation observations or prior information) is as small as possible. Often these regularisation constraints take the form of a homogeneity condition, ie. a constraint that differences between various pairs of parameter values (or their logs) be zero if possible. Thus, when used in regularisation mode with these constraints applied, PEST is asked to estimate a parameter set that deviates from uniformity only to the extent required to ensure a good fit between model outcomes and field data. Because the optimised parameter set is then defined not just in terms of its ability to allow the model to match field data well, but also in terms of its ability to replicate some “ideal” condition, solution to the inverse problem is often unique. This results in stable PEST behaviour and, if regularisation constraints are properly defined, a parameter set that is intuitively and geologically pleasing.

Pilot point programs supplied with the Groundwater Data Utilities allow regularisation constraints to be applied in two different ways. In both cases parameter relationships are defined using prior information equations that attempt to constrain parameter differences between nearby pilot points to zero. However the two methods differ slightly in the manner in which weights are assigned to the prior information equations that specify these conditions. In the first method all weights are the same. In the second method the weight assigned to each prior information equation which expresses the desirability of zero parameter difference between two particular pilot points is inversely proportional to the value of the kriging variogram calculated for the separation distance between these two pilot points. This method of weights calculation is justified by equation (5.5) and the fact that, ideally, observation and prior information weights should be equal to the inverse of their respective standard deviations (standard deviation is the square root of variance). Hence calculation of weights by this method has a sound geostatistical basis.

As is described in the documentation to PEST-ASP, PEST multiplies all weights assigned by the user to regularisation observations and prior information equations by a uniform “weight factor” which preserves the relative weighting between all such items. PEST calculates the weight factor itself in such a way as to ensure that the contribution of regularisation information, taken as a whole, to the objective function is not raised above the level where imposition of regularisation constraints erodes the

capacity of the model to fit the field data. The maximum tolerable level of model-to-measurement misfit is supplied by the user as part of PEST's data requirements when used in regularisation mode.

5.7 Predictive Analysis

In some ways, use of PEST in predictive analysis mode is similar to its use in regularisation mode in that PEST is asked to recognise a constraint at the same time as it attempts to ensure as good a fit as possible between model outcomes and field measurements. However when used in predictive analysis mode, the constraint is that a key model prediction be maximised or minimised while the model remains in a calibrated state. Thus use of PEST in predictive analysis mode often requires that the "model" as run by PEST actually consists of two instances of the model - one running under calibration conditions and one running under predictive conditions. (Note, however, that it is not always necessary that this be the case; if a "prediction" is defined broadly as some function of the model parameters, then calculation of this function may not actually involve another model run.)

The use of pilot points in model parameterisation as part of a predictive analysis exercise can be very useful when simulating subsurface contaminant transport. The fate of a contaminant is particularly sensitive to "geological fine detail". Unfortunately, it is rarely possible to resolve this fine detail during a calibration process based only on head and flow measurements. Although the use of borehole contaminant concentration or travel time measurements can assist in this regard (where MT3DMS or MODPATH is run jointly with MODFLOW to form the overall composite model run by PEST), rarely, if ever, will "parameterisation fine detail" be sufficiently well determined to prevent a large margin of error from being associated with predictions of contaminant fate. Hence, if computer modelling is to be used to maximum advantage in simulating contaminant transport processes under a particular site, the extent of uncertainty associated with contaminant fate predictions should be explored as part of the modelling process.

The use of pilot points to characterise the hydraulic property distribution of a model domain brings far more flexibility to the predictive analysis process than the use of zones. When calibrating a model on the basis of historical data in such a way that a particular prediction related to contaminant fate is maximised or minimised, the use of pilot points (especially if there is a superfluity of these points) allows PEST to define hydrogeological structures within the model domain that allow the full range of fate scenarios to be explored. Homogeneity constraints on parameter distributions can be imposed just as in regularisation mode in order to maintain hydrogeological realism; however PEST cannot adjust the weight factor assigned to these constraints while simultaneously maximising or minimising the key model prediction. However if predictive uncertainty is explored using the "dual calibration" method documented in the PEST manual, then it is possible to run PEST in regularisation mode while, at the same time, examining model behaviour under both calibration and predictive conditions simultaneously.

5.8 Utility Programs

5.8.1 General

A full description of each of the programs available through the Groundwater Data Utilities for pilot-point-based parameterisation is presented in Part B of this manual. However a brief overview is presented in this subsection.

5.8.2 PPK2FAC

PPK2FAC creates an “interpolation factor file” listing the kriging factors pertaining to each cell within the model grid to which interpolation is required; these are the factors by which interpolated hydraulic property values are calculated at cell centres based on the hydraulic property values assigned to the pilot points. Pilot point locations, together with initial property values to be assigned to these points at the commencement of the parameter estimation process, are supplied in a “pilot points file” - see Section 2.12 of this manual. Each pilot point is also assigned a zone number; this number must correspond to a number appearing in a “zonation integer array” which is used to specify the spatial disposition of each zone.

For each zone defined in the integer array, the user is asked to supply a “geostatistical structure”. As discussed above, a “geostatistical structure” is comprised of one or more nested variograms and an optional nugget. Variograms and structures are supplied through a “structure file” (easily prepared by the user); such a file is depicted in Section 2.20 of this manual, and described in detail as part of the documentation to program PPK2FAC. The user must also supply a number of other items of information which guide the way in which kriging is implemented within each zone of the model domain based on the pilot points assigned to that zone and the geostatistical structure associated with that zone.

As well as creating an interpolation factor file, PPK2FAC also creates a “standard deviation array file” and a “regularisation information file”. The former contains a MODFLOW-compatible real array depicting the square root of the kriging variance associated with each grid cell centre to which interpolation takes place. This can be imported into any MODFLOW GUI which supports array importation for graphical inspection. (There it will be seen that interpolation standard deviations are small near pilot points and much higher in between them.) The “regularisation information file” produced by PPK2FAC is used by program PPKREG to add regularisation constraints to a PEST control file based on the geostatistical information contained in the structure file. It contains the value of the nested variogram pertaining to every pair of pilot points that are used simultaneously for interpolation to one or more cell centres. Thus no “inter-zone” entries are recorded, and no entries are recorded for pairs of pilot points which are “too far apart” as defined by the user-supplied kriging search radius. This information is used in the calculation of relative weights assigned to prior information items which enforce the homogeneity constraint used for parameter regularisation when using PEST in regularisation mode.

5.8.3 FAC2REAL

Once kriging factors have been calculated, spatial interpolation can be undertaken. This is most easily accomplished using program FAC2REAL. FAC2REAL generates a MODFLOW-compatible real array on the basis of values assigned to pilot points, and the kriging factors generated by PPK2FAC. Once the array has been generated and stored in a file, it can be imported into a MODFLOW GUI for graphical inspection.

To use PEST for pilot-point-based calibration, two paths can be taken. In the first path, a “composite model” can be built (encapsulated in a batch file) comprised of FAC2REAL, followed by MODFLOW, followed by a postprocessor such as MOD2OBS and/or BUD2SMP to spatially and temporally interpolate MODFLOW outputs to the sites and times of field measurements. If necessary, the composite model can include MT3DMS and another incidence of MOD2OBS in order to allow concentration measurements to be used in the calibration process. Program PESTPREP can be used to assist in PEST input file preparation for calibration of this composite model (see Section 4.14 of this document for more details). For parameter definition, a template file would be built, based on the pilot points file; PEST would assign a property value to each such point prior to each model run. The MODFLOW-compatible array generated by FAC2REAL on the basis of each updated set of parameters could be “pasted” into the MODFLOW input dataset (for one or more layers) using program REPARRAY, or it could be accessed by MODFLOW using its “OPEN/CLOSE” functionality for the reading of external data arrays. If necessary, it would be no trouble to generate a number of different arrays in this manner, each based on different sets of pilot points, and each using different geostatistical structures for hydraulic property characterisation; these arrays could then be used to store the values of different hydraulic property types over the model domain, for one or many layers or hydrogeological units. Alternatively, different arrays could be based on the same set of kriging factors and pilot point locations, but on different values assigned to the same set of pilot points for definition of different property types, or of the same property type applied to different layers or hydrogeological units.

5.8.4 FAC2MF2K

The second option available for pilot-point-based groundwater model calibration is to modify an existing MODFLOW-2000 input dataset to incorporate pilot point parameterisation. This can be accomplished through program FAC2MF2K. Using this utility, (together with an easily-prepared “parameter replacement file - see Section 2.21 of this document and the documentation of program FAC2MF2K in part B of this manual), a user is able to remove certain parameters from an existing MODFLOW-2000 input dataset, replacing them with pilot-point-based parameters. MODFLOW-2000 *zone* and *multiplier* files are also modified, with new multiplier arrays added to the latter file based on kriging factors calculated by PPK2FAC; redundant arrays are also removed from these files. Thus, after FAC2MF2K has done its work, MODFLOW-2000 can be used in order to estimate hydraulic property values at pilot point locations (or, better still, the MODFLOW2000-to-PEST

translator can be used to translate the MODFLOW input dataset to PEST format, and PEST-ASP can be used to calibrate the model). Hence a modeller can use a commercial MODFLOW-2000 interface to set up his/her model (including observations to be used in the calibration process), incorporating a simple spatial parameterisation scheme based on uniformity or a small number of zones. Once the GUI has generated a set of MODFLOW-2000 input files pertinent to this problem, these files can be automatically modified by FAC2MF2K in order to replace the simple, zone-based parameterisation scheme with the pilot-point-based scheme.

Unfortunately, MODFLOW-2000 has some serious shortcomings when it comes to pilot-point-based calibration. As was mentioned above, spatial variation of hydraulic conductivity and transmissivity is often best described by a log-variogram rather than by a variogram pertaining to native hydraulic conductivity and transmissivity values. Spatial interpolation of these parameter types should thus be carried out on the basis of the logs of their values, rather than on the basis of the values themselves. This option is available when using program FAC2REAL described above. However this option is not available through MODFLOW-2000. Furthermore, as was also discussed above, it is often necessary that (location-dependent) upper and lower limits be placed on spatially-interpolated hydraulic property values; this prevents the occurrence of spurious values (including negative values if log-interpolation is not performed) that can sometimes occur as an outcome of the kriging process, especially if pilot points are too close together and a Gaussian variogram is employed. Such upper and lower interpolation limits can be readily applied by FAC2REAL when it is used to generate a MODFLOW-compatible real array. However there is no capacity within MODFLOW-2000 to apply these limits.

Fortunately, MODFLOW-2000 has been modified to overcome these problems. These modifications are such that logarithmic parameter interpolation can take place, and that upper and lower interpolation limits can be applied. However while these modifications allow MF2KASP (the modified version of MODFLOW-2000) to run in “forward mode” to calculate its usual set of outputs, including model-generated equivalents to field measurements, it cannot be run in *sensitivity* or *parameter estimation* mode when logarithmic interpolation is applied. This is because MODFLOW hydraulic property array values are no longer linearly related to actual parameter values under these conditions, thus violating a fundamental premise upon which MODFLOW-2000 *sensitivity* (and hence *parameter estimation*) functionality is based.

Fortunately these problems do not prevent the use of nonlinear parameter estimation in the MODFLOW-2000 context. Once a MODFLOW-2000 input dataset has been modified to include pilot-point-based parameterisation (whether or not this includes logarithmic interpolation), this dataset can be easily translated to PEST format using the MODFLOW-to-PEST translator MF2EST (see Doherty, 2001b); PEST can then be used to carry out the nonlinear parameter estimation process. This brings with it two advantages. The first is that PEST’s numerical performance is generally better than that of MODFLOW-2000 when calibrating highly parameterised systems. The second is that PEST can be used in regularisation or predictive analysis mode if

desired, thus allowing the full potential of pilot-point-based parameterisation to be realised in the calibration process; these options are not available in MODFLOW-2000. It should be noted however, that if logarithmic parameter interpolation is carried out, PEST must calculate parameter derivatives itself using finite parameter differences rather than relying on MF2KASP to calculate these derivatives through its *sensitivity* process. This is accomplished simply by setting the IMDERCALC variable to 0 when running the MODFLOW2000-to-PEST translator; see Doherty (2001b). The MODFLOW solution convergence criterion HCLOSE must also be set tighter than normal.

5.8.5 PPKREG

It is apparent from the above discussion that a PEST input dataset can be generated in one of two ways. It can be generated directly by the user (possibly with the help of PESTPREP, MOD2OBS, etc - see Section 4.14 of this document) using the first of the above alternatives, or it can be generated using a second, more circuitous, route comprised of (i) first generating a MODFLOW-2000 input dataset based on a simple parameterisation of the model domain, (ii) modifying this dataset to include pilot points using program FAC2MF2K, and (iii) converting this problem to PEST format using the MODFLOW2000-to-PEST translator MF2PEST. Irrespective of which of these two routes is taken, regularisation information can be incorporated into the parameter estimation process using a utility program named PPKREG. PPKREG reads an existing PEST control file in which at least some parameters are defined using pilot points. Then, based on the information contained in the “regularisation information file” generated by PPK2FAC, it adds a suite of prior information to the existing PEST control file, as well as a “regularisation” section. Each prior information equation added to the file states that the difference between parameter values assigned to two pilot points (or the logs of these parameter values if they are log-transformed during the parameter estimation process) should be zero. The same weight can be applied to all such prior information equations if the user desires; alternatively, weights can be calculated as inversely proportional to nested variogram values based on pilot point separations, using the same geostatistical structures employed in calculating the kriging factors. The latter methodology is intuitively more appealing, for the strength with which the homogeneity constraint is applied diminishes with distance of separation of the pilot points. Also, where a “search radius” or “maximum number of points” specification is used in the generation of kriging factors in order to limit the number of pilot points that are used in spatial interpolation to any one model cell centre, this is reflected in the specification of the uniformity constraints applied through the regularisation process. This serves to restrict the number of articles of regularisation prior information used in the inversion process to a manageable level. Thus if points are “too far apart” there is no prior information equation specifying that the preferred parameter difference between these two points should be zero.

Note also that because different sets of pilot points are used to undertake spatial interpolation in different zones, pilot points within different zones are not linked by prior information equations. Thus where the use of parameter zones is combined with

the use of pilot points, the effect of pilot-point-based regularisation is to constrain property variation inside each zone to a minimum, allowing property variation across zone boundaries to supply the degree of heterogeneity required in a model domain if the model is to calculate outputs which match field observations well. However if such a scheme does not supply the degree of heterogeneity required for a good model calibration to be achieved, internal zone heterogeneity will be introduced automatically through the parameter estimation process (only where necessary, due to imposition of regularisation constraints) to reduce the model-to-measurement misfit to a user-specified level.

Before using PEST in regularisation mode, the user should carefully read the pertinent section of the documentation to PEST-ASP. If regularisation is not properly applied it will not work. Basically, if parameter regularisation is used at all, it should be used pervasively.

5.9 MF2KASP

MF2KASP is documented in Doherty (2001b). It is a version of MODFLOW-2000 to which certain alterations have been made in order to optimise its performance when used with PEST. These alterations include the following:-

- MF2KASP writes a “derivatives file” containing the derivative of every model-generated-observation-equivalent with respect to every parameter. PEST uses this information to save it from having to calculate derivatives itself on the basis of repeated model runs using finite parameter differences;
- MODFLOW file output can be reduced substantially as PEST runs it repeatedly as part of the model calibration process;
- minor alterations have been made to the “book-keeping” attached to the declaration of “dry cells”;
- cells in the basal layer of a model domain can be prevented from going dry by retaining a “residual saturated thickness”; this can circumvent some of the problems that accompany operation of MODFLOW (particularly in a parameter estimation context) under conditions of limited recharge, and/or steeply dipping bedrock;
- alterations have been added to remove certain impediments to MODFLOW-2000’s ability to be used in conjunction with pilot-point-based parameterisation.

MF2KASP contains functionality that has been added specifically to enhance its performance when parameterisation is undertaken on the basis of pilot points. Activation of this functionality depends on settings supplied in an “*asp* input file”. If this file is not supplied to MF2KASP, then its performance is exactly the same as that

of the normal, USGS version of MODFLOW. Alternatively, if it is necessary for MF2KASP to read such a file in order that its PEST interface functionality be activated, that its internal array construction functionality be modified in order to better cope with pilot-point-based parameterisation, or to alter some other aspect of its functionality as listed above, then the name of the *asp* input file must be supplied in the MODFLOW name file for the current case. An entry such as that shown in Example 5.1 is thus required in the name file.

ASP 59 mf2k.asp

Example 5.1. Entry in a MODFLOW-2000 name file activating the *asp* process.

The “code” which activates the “*asp* process”, and thus ensures that MF2KASP reads an *asp* input file, is “asp”. Thus if a MODFLOW-2000 name file includes a line containing this “code”, followed by a unit number, followed by the name of text file containing input data for this process, then MF2KASP will read the *asp* input file, using the variables contained therein to modify the manner in which it calculates certain hydraulic property arrays based on parameters pertaining to those arrays. Note that the unit number appearing in example 5.1, though it must be present, is not important; MF2KASP finds an available unit number itself with which to open the file. Note also that program FAC2MF2K generates this file itself (and modifies an existing MODFLOW-2000 name file to include the reference to the *asp* input file) as part of its task of modifying a MODFLOW-2000 input dataset to include pilot-point-based parameterisation.

The specifications of an *asp* input file are provided in Example 5.2. Note that on most occasions of MF2KASP usage, the *asp* input file is written automatically by the MODFLOW-2000 to PEST translator MF2PEST (see Doherty, 2001b), or by program FAC2MF2K, and hence does not need to be prepared by the user. Furthermore, an *asp* input file written by FAC2MF2K is automatically modified by MF2PEST to ensure a smooth interface between MF2KASP and PEST when MF2PEST builds a PEST input dataset from a MODFLOW-2000 input dataset that has been modified for the use of pilot points by FAC2MF2K.

```

IPESTINT  INTERP
NOSTOP   HDRYBOT  LIMOP  MINTHICK

The following line is required if IPESTINT is set to 1.
PESTCTLFIL

All of the following lines are required only if INTERP is set to 1.
NUMPARTYPE  NUMARRAY

Repeat the following line NUMPARTYPE times
PARTYP  INTERPTYP  MININTERPVAL MAXINTERPVAL (LAYER(I), I=1,NLAY)
or
PARTYP  INTERPTYP  MININTERPVAL MAXINTERPVAL (PERIOD(I), I=1,NPER)

Repeat the following two items NUMARRAY times
ARRAYNAME
ARRAY

```

Example 5.2. Specifications of an *asp* input file.

An example of an *asp* input file in which no alterations are made to internal MODFLOW array generation functionality to accommodate the use of pilot points is shown in Example 5.3. As is apparent from a comparison with Example 5.2, this file is much shorter than it has the potential to be. This is because no variables are required in this file governing alterations to MODFLOW-2000 parameter manipulation functionality as INTERP (on the first line of this file) is set to 0 signifying de-activation of enhancements pertaining to internal array calculation. However if INTERP is set to 1, then a suite of other data must be supplied in the *asp* input file which governs the manner in which MODFLOW calculates arrays from parameter values.

```

1      0                                IPESTINT  INTERP
1      0      1      0.00000          NOSTOP    HDRYBOT  LIMOP  MINTHICK
pestrun.pst                          PESTCTLFIL

```

Example 5.3. Example of an *asp* input file with INTERP set to zero.

The role of each of the variables cited in the first two lines of Example 5.2 will not be discussed, as they are discussed elsewhere - see Doherty, 2000b. It should be noted, however, that if each IPESTINT, INTERP, NOSTOP, HYDRBOT, LIMOP and MINTHICK are set to zero, then behaviour of MF2KASP is identical to that of MODFLOW-2000.

Example 5.4 shows part of an *asp* input file in which INTERP is set to 1. If INTERP is set to 1, then values must be supplied for a number of variables which govern modifications to MODFLOW array-computation on the basis of parameter values. These variables are now described; refer to Example 5.2 for the locations of these variables in the *asp* input file.

```

0      1                                IPESTINT  INTERP
1      0      1      0.00000          NOSTOP      HDRYBOT      LIMOP      MINTHICK
3      2                                NUMPARTYPE NUMARRAY
HK          1  ARRAY1          1.0e2          1  1  0
SY          0  0.05          ARRAY2          0  0  1
RCH         0  1.0E-7          1.0E-3          1  1
ARRAY1
1.000000  1.000000  1.000000  1.000000  1.000000
1.000000  1.000000  1.000000  1.000000  1.000000
1.000000  1.000000  1.000000  1.000000  1.000000
.
.
ARRAY2
0.20  0.20  0.20  0.20  0.20  0.20  0.20  0.20  0.20
0.20  0.20  0.20  0.20  0.20  0.20  0.20  0.20  0.20
0.20  0.20  0.20  0.20  0.20  0.20  0.20  0.20  0.20
.
.

```

Example 5.4. An *asp* input file for which INTERP is set to 1.

NUMPARTYPE

NUMPARTYPE is the number of parameter types referenced in the following lines of the *asp* input file. Each parameter type cited in this file must be suitable for use by the MODFLOW-2000 *lpf* or *rch* package; possible types are ‘hk’, ‘hani’, ‘vkcb’, ‘vk’, ‘vani’, ‘ss’, ‘sy’ and ‘rch’.

NUMARRAY

NUMARRAY specifies how many arrays are listed in the *asp* input file. These arrays, if present, specify cell-specific array upper and lower bounds after spatial interpolation has been carried out using kriging factors encapsulated in MODFLOW multiplier arrays.

PARTYP and INTERPTYP

NUMPARTYPE lines of data must follow the line in which NUMPARTYPE and NUMARRAY are specified, each containing $4 + nlay$ items or $4 + nper$ items, where *nlay* is the number of layers pertaining to the current model and *nper* is the number of stress periods. The first entry on each of these lines (PARTYPE) is the name of an *lpf* parameter type or *rch* parameter type (of which “rch” is the only allowed type). The next entry (INTERPTYP), an integer, must be 1 or 0. If it is 0, then internal MODFLOW hydraulic property array construction is undertaken by summing parameter values multiplied by elements of the multiplier arrays in the normal MODFLOW-2000 manner. However if it is supplied as 1, then the elements of property arrays are calculated by summing the logs of parameter values, and then raising the summation to the power of 10. Where multiplier arrays are generated by

FAC2MF2K on the basis of kriging factors, this is equivalent to kriging on the basis of log parameter values.

MININTERPVAL and MAXINTERPVAL

The next two entries on these lines, (viz. MININTERPVAL and MAXINTERPVAL) can be either numbers or names. If the first of these entries is a number, then it represents the minimum value that the pertinent hydraulic property can take over the area of the model domain. However if the entry is not a number then it is assumed to be an array name. In this case minimum hydraulic property values are cell-specific and are read from the named array. Similar considerations apply to MAXINTERPVAL, which provides the maximum allowable interpolated hydraulic property value.

LAYER(I) or PERIOD(I)

Each of the final *nlay* or *nper* entries must be either 1 or 0. Each entry pertains to a particular model layer (if the parameter is of *lpf* type) or to a particular stress period (if the parameter is of *rch* type); counting of layers begins at the surface. If the entry for a particular layer or stress period is 0, then data provided previously on this line is inapplicable to that layer or stress period; if it is 1, then values supplied for INTERPTYPE, MININTERPVAL and MAXINTERPVAL are all applicable to that layer or stress period.

Note that different lines within the first section of the file can cite the same property type (ie. PARTYP). This may occur if the interpolation specifications are different for different layers, or different stress periods, in the model.

ARRAYS

Then follow NUMARRAY arrays. The dataset provided for each array is comprised of the array name, followed by the array itself. Note that the normal MODFLOW protocol for array input is not followed, in that each array is not preceded by a header line in which formatting specifications are provided. Thus the array cannot be read using the MODFLOW array reading utility subroutine U2DREL.

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