

COMPUTER TECHNIQUES
IN GROUNDWATER RESOURCES
STUDIES

Reference Manual

June 1979

SUMMARY

This reference manual is concerned with a computer data system developed specifically for groundwater studies. The system has been designed to analyse data from regional studies, where some impact can be made using scientific methods coupled with efficient data retrieval. It is not intended for large scale, long-term data archival.

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KEY TO FIGURES AND TABLES

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NOMENCLATURE

- Program names capitals, underlined (e.g. CONTROL)
- Control words capitals (e.g. NEW-SYSTEM)
- Data system files enclosed in square brackets (e.g. [Site-list])
- All options are in italics (e.g. [*Type 1*] refers to an example
data file or *qual*filename* refers to a mass
storage file.)

BIBLIOGRAPHY

- (1) Computer Techniques in Groundwater Resource Studies - First Interim Report, July 1978.

Computer techniques offer a basic facility to handle and analyse large quantities of data. One of the main aims of this project has been to develop general analytical methods which can be applied to groundwater resource studies.

- (2) Using the Groundwater Data Forms, March 1979

Data collected during groundwater resource studies can conveniently be written onto coding forms in the field. The coding forms have been designed in such a way as to minimise the number of different types of forms and also lead to data being put directly onto the computer in a simple efficient way. Data not falling into either the data categories or the descriptions discussed in this text can be entered on the coding forms and also on to the data system as long as some preparation work is done beforehand.

- (3) Computer Techniques in Groundwater Resource Studies - Second Interim Report, August 1979

Examples of data from two hydrogeological studies have been used to illustrate some of the computer techniques which are now available. They have been grouped into the different data categories and, in conjunction with the reference manual, will help the users to operate the system. In addition it is hoped that they will stimulate ideas for useful additional techniques.

CHAPTER 1 - General considerations

The reader is referred to the references listed in the bibliography for a description of the motivation and the structure of the data system (1), the use of the groundwater coding forms (2), and for examples of those analytical facilities which have already been developed (3). This report is solely concerned with operating the system on the N.E.R.C. Univac 1108 computer. It describes how to put data onto the system, quality control of data, selection of relevant parts of the data, correcting data and hydrogeological data analysis. Appendices A and B contain descriptive lists of control words and error messages and appendix C a number of specific points which should be noted before attempting to set up the data system for a particular study.

A control program has been developed to simplify the operation of the system. The program accepts simple control words and generates the relevant computer runstream. It is possible, although more complicated, to operate the system without using the control program; however this is beyond the scope of this report.

In order to use the data system with the control program, the following cards are required

@RUN *runid, account, qualifier*¹

@XQT ODM,CONTROL.CONTROL

*Control cards*²

*Data cards*³

@FIN

Notes ¹. The parameters on the RUN card are:

runid - an identifier for the particular run, chosen by the user

account - the account number assigned to the project

qualifier - the qualifier assigned to the project

All work concerned with a particular project should be run under a unique qualifier. This enables the data system to identify those files which relate to a project and also protects against overwriting files from another project. Obviously no two projects should use the same qualifier and before starting a data system, with a new qualifier, users should check that the qualifer is not already being used (see Appendix C).

Each control card has a 'control word' in the first 12 character locations of the card and may contain further information in the remaining 68 locations; additional information may be contained on continuation cards (see Appendix A).

The first control card will always be a TITLE card, which has a project title in locations 13-36; this title will appear on all output generated by the system and thus should remain constant throughout the study. The last control card will always be ENDRUN.

These data cards are needed only if data is to be added to the system in the form of a set of punched cards rather than a mass storage file (see Chapter 2: Putting Data onto the System).

The program CONTROL generates the runstream required to perform the desired manipulations of the data; if no errors are detected, the program will

usually cause this runstream to be executed. However if a HOLDRUN card is included, it will cause the program to list the control cards and the runstream generated; this runstream will not be executed. A copy of this runstream may be kept on file by specifying a file-name in columns 13 to 36 of the HOLDRUN card. If an error is detected, a list of the control cards and of the runstream generated before the error was detected will be printed, together with a diagnostic message.

	HOLDRUN	not HOLDRUN
Success	Message: successful execution of CONTROL. Lists control cards Lists runstream generated. Writes runstream to file (if specified on HOLDRUN card).	Message: successful execution of CONTROL; job now running. Lists control cards.
Failure	Message: error - Diagnostic <i>xx</i> (where numbers <i>xx</i> are listed in Appendix B) Lists control cards read in before error detected. Lists runstream generated before error detected.	

Table 1. Control program status

CHAPTER 2 - Data

2.1 Coding the data.

Data of standard types (see Table 2.) can most conveniently be put onto the system if they have been recorded on the groundwater data forms (see "Using the Groundwater Data Forms" for details of the layout and use of the forms).

Filename	Type	Page reference to 'Using the Groundwater Data Forms'
SITE-LIST	Master	
LITHOLOGY	Library	11
CHEMISTRY	Master	13
PUMPING-TEST	Library	16
WATER-LEVEL	Library	18
CONDUCTIVITY	Library	20
TEMPERATURE	Library	22
LOG-COND	Library	24
LOG-TEMP	Library	26

Table 2. Standard data types

The data from these forms are punched onto cards. In the case of data which will be stored on master-files (i.e. [Site-list] and [Chemistry] data) the data cards must be preceded by a set of cards describing the particular format that has been used - these can be punched directly from the information which has been entered on the key form for the particular data-types. Note that locations 78-80 of the last card describing the format must contain 'END' to enable the program to differentiate between the key and the data.

In our experience, it is advisable to read the cards into a mass storage file before adding them to the system, since it is then simple to correct errors using the editor (@ED processor).

2.2 Checking for format errors

The formats for the standard data types can be checked using the program CHECKFORM - this checks that the format is compatible with that expected by the data system. A successful execution of CHECKFORM ensures that the data will be read successfully by the system, although there could still be errors in the data. Five cards are required to run the program:

```
@RUN runid, account, qualifier
@XQT ODM*CONTROL.CHECKFORM
data-type1
@ADD qualifier*filename2 (or data cards)
@FIN
```

Notes. *data type* is the name of the standard data type (Table 1),
left-justified in the first 12 locations.

2. *qualifier*filename* is the qualifier and filename of the
mass storage file to which the data has been written. If the data is
on cards rather than in a mass storage file, this card (@ADD *qualifier*
filename*) is removed and replaced by the set of data cards.

The message "FORMAT CHECKED FOR [*Data-type*] DATA - ALL RIGHT TO ADD
TO DATA SYSTEM" indicates a successful execution of CHECKFORM.

Should CHECKFORM be unsuccessful, then either the data-type has not
been recognised or there is an error in the format of the data. CHECKFORM
gives some indication of where the first error was found. There may be
format errors later on in the data which can only be detected once the
earlier errors have been corrected.

If CHECKFORM has been unsuccessful then the effect of trying to put the
data onto the system is unpredictable and may result in losing or
corrupting data which is already on the system.

If the data are in a mass storage file then it is possible to run CHECKFORM as a demand job from a terminal and use the editor to correct errors as and when they are detected. If there are a number of errors then the savings in time can be considerable.

2.3 Putting the data onto the system.

Data is added onto the system using the control language. The control cards which are required in a given situation can be determined from the flow diagram (Fig 1). The following cards are required

@RJN *runid, account, qualifier*

@XQT ODM*CONTROL.CONTROL

Control cards

Data cards

@FIN

Example sequences of control cards, and the circumstances in which they are used are given below.

In the examples [*Type 1*], [*Type 2*], etc represent the names of standard data types (see Table 1), while *qual,*file A*, *qual,*file B*, etc represent the qualifiers and filenames of the mass storage files containing data to be added to the system.

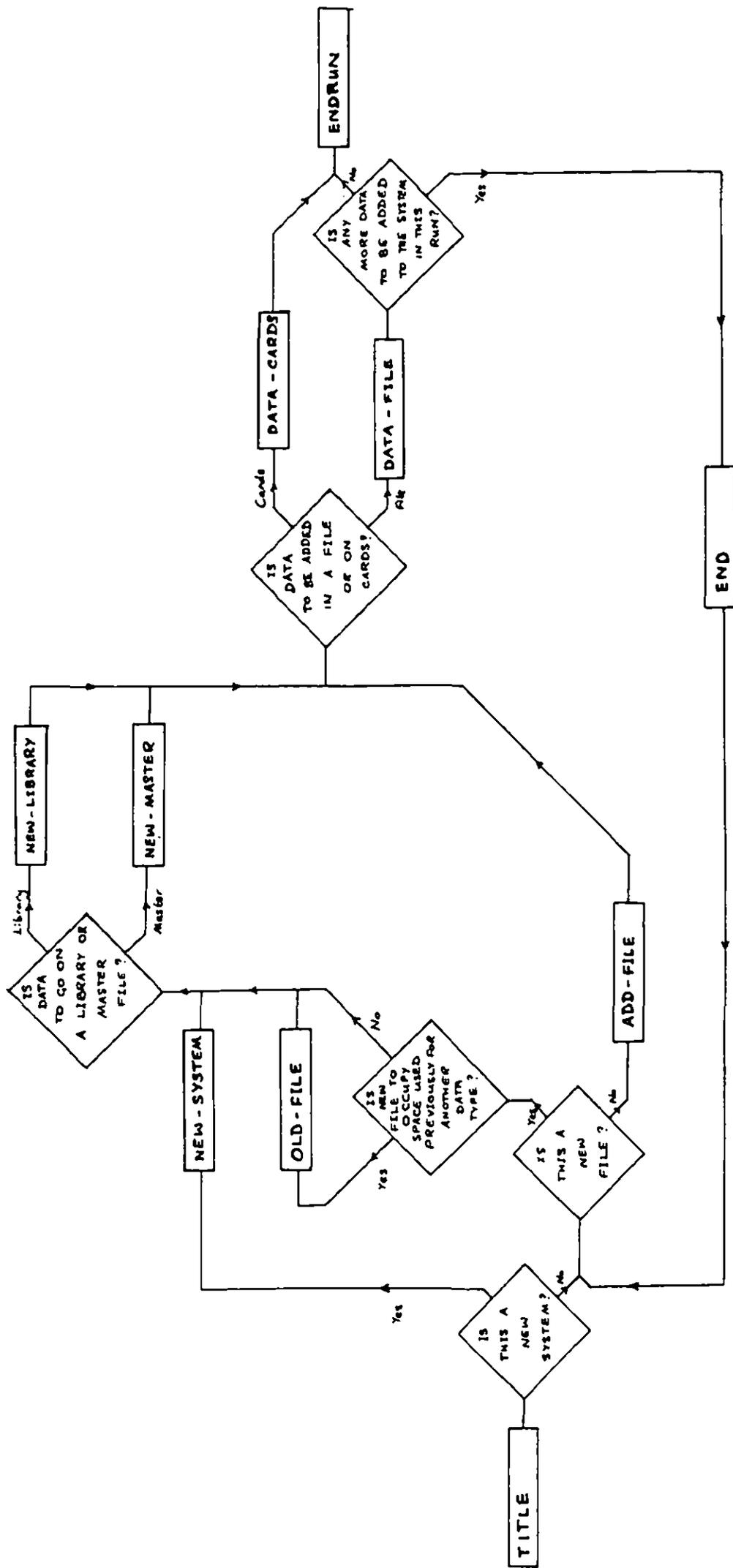


FIGURE 1. Control words (see Appendix A) required to add data to the system.

Example 1. Initial run - starting a new system (with a library file)

```
TITLE      project title
NEW-SYSTEM
NEW-LIBRARY [Type 1]
DATA-FILE  qual,*fileA
ENDRUN
```

This example assumes that [Type 1] represents one of the standard data types for which the data is stored on a library file - for those types which are stored on master files, NEW-LIBRARY is replaced by NEW-MASTER as in example 2.

Example 2. Opening a new file - system already exists (for a master file)

```
TITLE      project title
NEW-MASTER [Type 2]
DATA-FILE  qual,*file B
ENDRUN
```

Example 3. Adding data to a file (library or master) which already exists

```
TITLE      project title
ADD-FILE   [Type 3]
DATA-FILE  qual,*file C
ENDRUN
```

Example 4. As long as the data to be added are in mass storage files, then more than one operation can be performed in one run. Suppose that data (in *qual,*file D*) is to be added to [Type 4] which has already been opened in a

previous run; and that a new library file [*Type 5*] is to be opened with data which is in *qual_{*}file E*. Then either of the following sets of control cards may be used, with identical results

TITLE	<i>project title</i>	TITLE	<i>project title</i>
ADD-FILE	[<i>Type 4</i>]	NEW-LIBRARY	[<i>Type 5</i>]
DATA-FILE	<i>qual_*file D</i>	DATA-FILE	<i>qual_*file E</i>
END		END	
NEW-LIBRARY	[<i>Type 5</i>]	ADD-FILE	[<i>Type 4</i>]
DATA-FILE	<i>qual_*file E</i>	DATA-FILE	<i>qual_*file D</i>
ENDRUN		ENDRUN	

Example 5. Adding data to an already existing file; data on cards.

```

TITLE      project title
ADD-FILE   [ Type 6 ]
DATA-CARDS
ENDRUN
Data cards

```

Example 6. If a particular data type [*Type 7*] is no longer required for a study, it may be over-written with a new data type [*Type 8*] (thus reducing the amount of storage space required).

```

TITLE      project title
OLD-FILE   [Type 7]
NEW-LIBRARY [Type 8]
DATA-FILE  qual*file F
ENDRUN

```

Example 7 Adding code details - for assigning values to the user-defined codes (numbers 1-11). See chapter 3 for an explanation of the use of codes.

```
TITLE      project title
ADD-CODE
DATA-FILE  qual*file G1
ENDRUN
```

Note 1. The data format is one card per grid reference as follows

$$\text{grid ref } /c_1 = v_1 / \dots /c_n = v_n /$$

where

$c_k, k=1\dots n$, are code numbers and the v_k are the corresponding values. The values of any codes which are not included in $c_1 \dots c_n$ are left unchanged, so for each station it is only necessary to specify those codes for which the values are to be changed.

Example 8. Keyfile information.

```
TITLE      project title
NEW-KEY
DATA-FILE  qual*file H1
ENDRUN
```

Note 1. The data format is as described in the "Using the Groundwater Data Forms" ..

CHAPTER 3 Selection

The station index contains the grid references of all the sample points, arranged in ascending order. The application programs work sequentially through the station index accessing and processing the data for each of the stations in turn. Analysis may only be required for the data from a few grid references, in which case it is wasteful to perform the analysis for all grid references in the station index. It is possible to select a subset of the station index (the selected station index) containing only those grid references which are of interest and to use that instead of the full station index.

There are two control words (SELECT and MAPSELECT) that can be used when making a selection, their use governed by the type of application programs; MAPSELECT must be used for programs which involve the plotting of maps (e.g. WL-DIFMAP, SITEMAP, etc). With both control words, columns 13-36 of the card should contain a description of the selection criteria; this appears together with the project title on the output.

The control card is followed by up to 15 criteria on which the selection will be based. There are 4 different classes of selection criteria as follows

1. CODE
2. BOX
3. QUAD
4. GRID

(The BOX and QUAD criteria may **not** be used in conjunction with MAPSELECT).

CODE

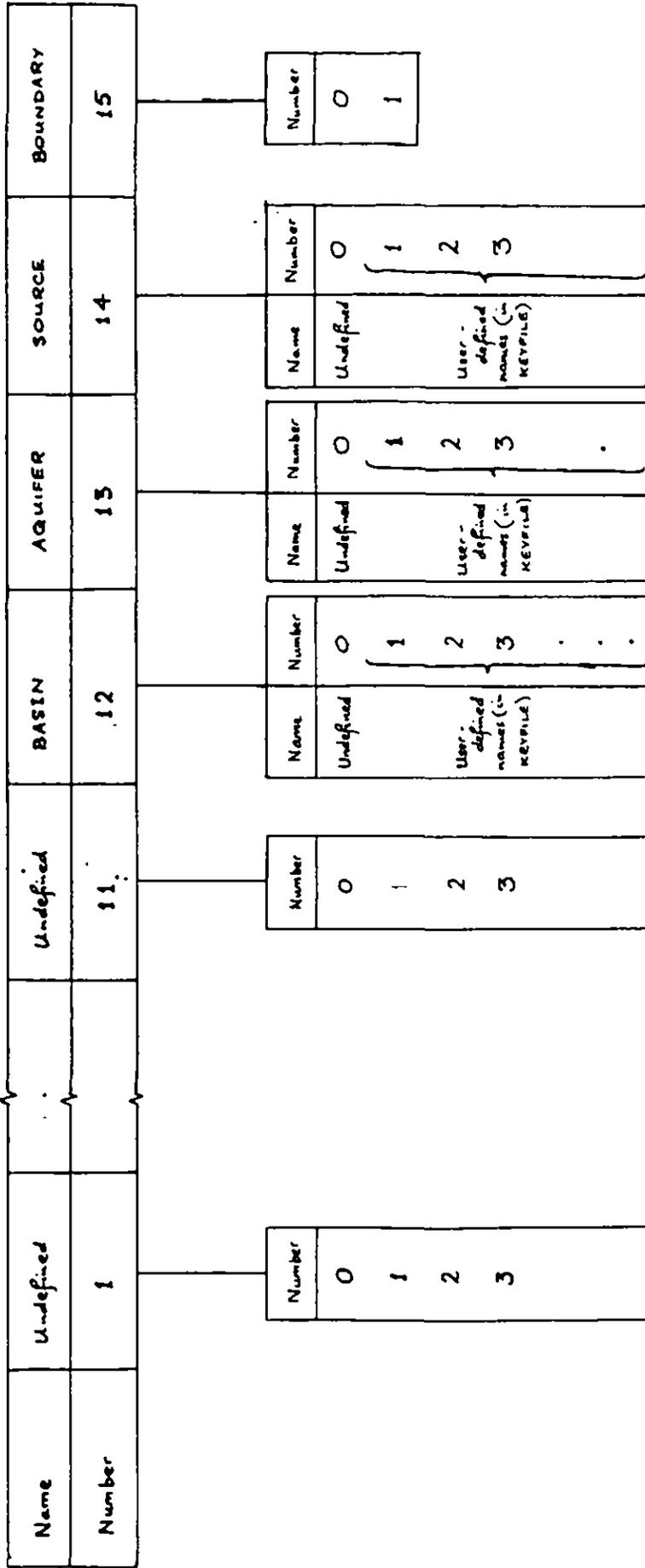
The codes are assigned values and thus group data with similar hydrogeological, physical or geographical characteristics. Grid references are selected, where these codes have certain values. The codes are identified by a number (1-15) and in the case of codes with the numbers 12-15 they have associated system defined names:

	<u>Number</u>	<u>Name</u>
Codes	12	Basin
	13	Aquifer
	14	Source
	15	Boundary

The values are also identified by a number and for codes 12-14 can have an associated user defined name (see Figure 2). Thus, for example, code number 14 (source) could have values; number 1 (Borehole), number 2 (Disused well) and number 3 (Spring) (see also "Using the Groundwater Data Forms"). For each station the values taken by codes 12-14 can be specified on the [Site-list] data form. Moreover, names associated with these values can be stored on the Keyfile (see 2.4).

The boundary code has the value 1 for those grid references for which there is boundary data; otherwise it has the value zero. The value 1 is assigned automatically when boundary data for that grid reference is added to the system.

For each grid reference all the codes have a default value of zero.



CODES.

VALUES.

FIGURE 2. Code names and numbers

QUAD. Each QUAD criterion is defined by one card: the format is

QUAD X1 = $x_1/Y1 = y_1/X2 = x_2/Y2 = y_2/X3 = x_3/Y3 = y_3/X4 = x_4/Y4 = y_4/$

This criterion is satisfied if the grid reference defined by co-ordinates (X,Y) is such that it falls in the quadrilateral whose vertices, numbered in an anticlockwise sense are (x_1, y_1) (x_2, y_2) (x_3, y_3) and (x_4, y_4) .

GRID

A GRID criterion is defined by a set of cards

GRID	(Card 1)
<i>grid-ref 1</i>	(Card 2)
⋮	⋮
<i>grid-ref N</i>	(Card N+1)

Grid references are selected if they appear (in columns 1-8) in the list (Cards 2 to N+1) of grid references. If a GRID criterion is included in any set of selection criteria, it must always be the last of the selection criteria included.

The end of a set of selection criteria is indicated by a card

END

Examples.

```
(i)  MAPSELECT  Selection criteria description
      CODE      12/1
      CODE      7/6
           BASIN/3

      END
```

This will give boundaries as well as grid references for which either
(a) code number 12 has value 1 or (b) code number 7 has value 6 and code name
BASIN (number 12) has value 3.

```
(ii) SELECT     Selection criteria description
      CODE      12/1
      CODE      7/6
           BASIN/3

      END
```

This will give the same selection as example (i) although the boundaries will
not be included.

```
(iii) SELECT     Selection criteria description
      CODE      12/3
      BOX       XMIN = 1046/XMAX = 1076/YMIN = 5230/YMAX = 5317/
      CODE      1/6

      END
```

This will give grid references lying in the rectangle

1046 < X < 1076 , 5230 < Y < 5317

for which either (a) code number 12 has value 3 or (b) code number 1 has value 6

```
(iv) SELECT      Selection criteria description
      GRID
      11535049
      10565215
      10635246
      END
```

This will give the three grid references in the list.

```
(v) SELECT      Selection criteria description
      CODE      12/3
      BOX      XMIN = 1046/XMAX = 1076/YMIN = 5230/YMAX = 5317/
      CODE      1/6
      GRID
      11535049
      10565215
      10635246
      END
```

This will give grid references selected in either example (iii) or example (iv). Note that the GRID criterion must come immediately before the END card.

The control word ENDSELECT ends the use of the selected station index and reverts to the full station index; a different selection can then be made, or work can continue using the full station index.

CHAPTER 4 - Quality control of data

For various standard types there are programs which search the data, in the system, for possible numerical error. (CHECKFORM described in Section 2.3 can only detect format errors and is used prior to putting data onto the system).

The different data types have certain general characteristics (for example, during each stage of a pumping test water levels are usually monotonic). The programs detect deviations from the general characteristics of the particular data types. The user must decide on whether or not the detected deviation is an error. The programs do not infallibly detect errors, since parts of the data may genuinely deviate from the characteristics of the data type causing spurious errors to be detected. Alternatively, errors may be missed because they are smaller than the detection tolerance.

By using the selection facility (Chapter 4) to select relevant stations, it is possible to apply a quality control program to only those grid references for which the data of a particular type has been changed.

The programs described in Chapter 6 can be used to produce data lists for visual checking.

The control word QUALITY is used to run the quality control programs; details of the additional parameters for particular data types are given in Appendix A.

(1) [Site-list] No quality control program. Use LOC-SUMMARY and SITE-SUMMARY (see Appendix A) to produce listings for checking.

(2) [Lithology] Checks that depths are in correct sequential order and that abbreviations used for components are compatible with those in the Keyfile

(3) [Chemistry] Calculates the percentage balance for each analysis, using the determinations for sodium, potassium, magnesium, calcium, sulphate, chloride, carbonate, bicarbonate and nitrate ions.

The domestic suitability is determined using criteria laid down in the "WHO International Standards for Drinking Water, 3rd Edition, 1971".

We have divided waters into Class 1, 2 and 3 on the basis of the following conditions:

CLASS 1 waters have all constituents below the WHO highest desirable levels.

CLASS 2 waters have all constituents below the WHO maximum permissible level but have one or more constituents exceeding the highest desirable level.

CLASS 3 waters have one or more constituents exceeding the maximum permissible level.

Agricultural suitability is based on the U.S. Salinity Laboratory System (U.S. Salinity Laboratory Staff 1954, Diagnosis and improvement of saline and alkaline soils: U.S. Dept of Agriculture Handbook No. 60) using the Sodium-Adsorption Ratio (SAR) and electrical conductivity (EC).

The electrical conductivity which is assumed to have been recorded at 20°C is corrected to the US standard at 25°C (ECL) by

$$ECL = \log_{10} (EC + 0.1 EC).$$

The salinity hazard classes are defined by

Range of ECL	Class
ECL < 2.398	C1
2.398 ≤ ECL < 2.875	C2
2.875 ≤ ECL < 3.352	C3
3.352 ≤ ECL < 3.699	C4
3.699 ≤ ECL	C5

The SAR is determined by

$$SAR = \frac{Na}{\sqrt{\frac{Ca + Mg}{2}}}$$

where the concentrations of Na, Ca and Mg are in milli-equivalents per litre. The sodium (alkali) hazard classes are then defined by

Range of SAR	Class
SAR < (-4.414 x ECL + 18.828)	S1
(-4.414 x ECL + 18.828) ≤ SAR < (-6.769 x ECL + 31.538)	S2
(-6.769 x ECL + 31.538) ≤ SAR < (-8.829 x ECL + 43.658)	S3
(-8.829 x ECL + 43.658) ≤ SAR < 31.	S4
31. ≤ SAR	S5

The values obtained for the balance and water class as defined above are added to the data on the [Chemistry] file for future use. It is possible, in addition to selecting for certain stations, to choose whether to quality control all chemistry samples or only those that have been changed, using one of the parameters on the control card.

(4) [Pumping-test] Checks that the number of steps is correct; and, in the case of a step drawdown test, that the steps are correctly ordered.

Generally the drawdowns from pumping tests will increase or decrease monotonically during each step. The program ascribes reversals of this trend to possible errors.

(5) [Water-level] Usually water levels vary smoothly; the quality control consists of identifying points which deviate from this smooth variation by more than a certain tolerance δ defined by the user. By running the program with several values of δ , a number of different sets of points with questionable values can be generated. A suitable set is then selected for detailed checking.

Details of the method are as follows. Suppose that for a particular station there are water level readings corresponding to n dates and $n \geq 4$ (if $n < 4$ no quality control is attempted); let the minimum and maximum levels be h_{\min} and h_{\max} . A cubic spline is fitted to the data, defined in terms of the values and gradients at the n dates. An estimate of the value of the k -th date is made using the values and gradients at the $(k-1)$ and $(k+1)$ dates; define the difference between this estimate and the actual value to be ϵ . The points are detected for which

$$|\varepsilon| > \delta (h_{\max} - h_{\min})$$

where δ is the user-defined tolerance.

(6) [Conductivity] No quality control program. Use CONDSUM to produce listings for checkings (see Appendix A).

(7) [Temperature] No quality control program. Use TEMPSUM to produce listings for checking (see Appendix A).

(8) [Log-cond] Checks that depths are in the correct sequence.

(9) [Log-temp] Checks that depths are in the correct sequence.

(10) Keyfile No quality control program. Use LIST-KEY to check on contents (see Appendix A).

CHAPTER 5 - Correction of errors

5.1 Standard data types.

Errors in the data, on the system, can be corrected using the control words LIST-FILE and EDIT-FILE in conjunction with the editor. LIST-FILE causes the data to be written to a specified unassigned mass storage file, where corrections can be made using the editor. The amended data from the mass storage file is replaced on the system using EDIT-FILE; after which the mass storage file is deleted. Consequently there are three stages to correcting errors for any standard data type, as follows:

- (i) Listing the data.

Execute CONTROL with the control cards

```
TITLE
SELECT      project title
             Selection
             criteria1
END
LIST-FILE   data-type2/qual*filename3
             Format
             details4
ENDRUN
```

Notes 1. The selection criteria are chosen so as to give only those grid references which require correction - usually by selection of individual grid references.

3. *data-type* is the name of the library or master file which requires correction and is always followed by a '/'

3. *qual*filename* is the name of the mass storage file to which the data is to be written - this must be an unassigned file.

4. *format details* are only required for master files - [Chemistry] and [Site-list].

(a) For [Chemistry] data, the LIST-FILE card should be followed by the names of the items which are to be written out, one per card. For example

```
LIST-FILE  CHEMISTRY/qual*filename
NA/2
CA/3
HCO3/2
END
```

This would cause the following to be written out for each station on the selected station index: Grid reference, sample number, followed by values for 'NA (to 2 decimal places), 'CA (3 d.p.) and 'HCO3 (2 d.p.). The number of decimal places should be chosen equal to the maximum precision of the determination. Determinations on the standard list are all written out as meq/l. - even if originally recorded as mg/l.

(b) For [Site-list] data the standard items which appear on the data forms are always listed. Additional items which have been added to the end of the file are included by listing their names; one per card. In the case of character

variables no further information is required. In the case of real variables the item name is followed by a '/' and the number of decimal places required, as in (a) above. For example

```
LIST-FILE  SITE-LIST/qual*filename  
PUMP TYP  
GROUND E/3  
END
```

where PUMP TYP is a character variable and GROUND E is a real variable whose values are printed to 3 decimal places. The last card must always be an END card, even if no additional items are required.

(ii) Editing and checking the data.

The format in which the data are written to the mass storage file corresponds to that used for each data type on the standard data forms. Obviously, the format of the amended data must similarly correspond. After using the editor to make the necessary corrections, CHECKFORM can be used to ensure that no new format errors have been inadvertently introduced.

(iii) Replacing the data.

Execute CONTROL with the control cards

```
TITLE      project title
EDIT-FILE  data-type/qual*filename
ENDRUN
```

where *data-type* and *qual*filename* are as above. The file *qual*filename* is deleted immediately after replacing the data - thus the same mass storage file can be used again for further corrections.

5.2 Changing the Keyfile.

Changes to the Keyfile can be made in one of two ways. In either case, the Keyfile will be completely re-written, so that all the relevant Keyfile information must be included each time that it is updated.

(a) The control words LIST-KEY and EDIT-KEY can be used in a similar fashion to LIST-FILE and EDIT-FILE:

(i) Execute CONTROL with the control cards

```
TITLE      project title
LIST-KEY   qual*filename1
ENDRUN
```

Note 1. *qual*filename* is the name of the mass storage file to which the contents of the Keyfile are to be written - this must be an unassigned file.

(ii) The editor can now be used to make the necessary amendments to the Keyfile data; as before the format is the same as on the standard data forms.

(iii) Execute CONTROL with the control cards

```
TITLE      project title
EDIT-KEY   qual*filename
ENDRUN
```

where "*qual*filename*" is as above.

The file "*qual*filename*" is deleted immediately after replacing the data.

(b) If substantial changes are to be made to the Keyfile it may be easier to complete a set of the standard Keyfile data forms and use the control word NEW-KEY as described in Chapter 2 (Example 8). This will overwrite the current version of the keyfile with the new version.

CHAPTER 6 - Application programs

The application programs described below are designed to display data which has been stored on the data system in a form which is suitable either as an aid to analysis or for inclusion in reports. Only a brief summary of the alternatives is given in this chapter; Appendix A contains an alphabetical list of control words, with details of any further information which must be included on the control cards. Examples of the output from these programs are given in the Second Interim Report.

6.1 Site-list data

- 6.1.1 LOC-SUMMARY Produces a summary showing, for each grid reference, the description of the site location as stored on the [Site-list] file.
- 6.1.2 SITE-SUMMARY Produces summaries of data on the [Site-list] file, five grid references per page, using either a standard format incorporating solely the standard list or the standard format with additional variables appended.
- 6.1.3 SITEMAP Produces a map showing the relative locations of the grid references for which there is [Site-list] data - the points are labelled with the reference name or number which appears in the first 10 characters of the site location.

6.2 Lithology data

6.2.1 LITH-LOG

For each grid reference, produces a lithological log from the data on the [Lithology] file. The abbreviations used for the lithology data which have been stored on the [Keyfile] are displayed on the log. If water level data exists for the borehole the minimum and maximum levels are marked together with levels reached whilst pumping, where appropriate.

6.3 Chemistry data

6.3.1 CHEM-SUMMARY

Produces summaries of data on the [Chemistry] file, five samples per page, using either a standard format incorporating the standard list of determinations, or the standard format with further determinations appended, or a format which is completely user-defined.

6.3.2 RATIO

Produces a summary of the values of up to six specified chemical ratios, for all samples.

6.3.3 STIFF

Produces a Stiff pattern diagram for each chemistry sample satisfying certain criteria, specified by the user.

- 6.3.4 PIPER Produces a tri-linear (Piper) diagram of chemistry samples for which the principle ions satisfy certain criteria. In addition, a summary giving the actual values of the determinations for these samples.
- 6.4 Pumping-test data
- 6.4.1 TEST-SUMMARY Summarises the [Pumping-test] data for each grid reference.
- 6.4.2 TEST-PLOT Produces graphs of drawdown against time of pumping for each pumping test; the user can specify either a log-log plot, or a log-linear plot, or both.
- 6.5 Water-level data
- 6.5.1 DW-SUMMARY Produces for each grid reference a summary of the depths to the water table, as recorded on the [Water-level] file.
- 6.5.2 WL-SUMMARY Produces for each grid reference a summary of the water levels (above mean sea level), using the datum which has been recorded on the [Site-list] - hence it is necessary that the [Site-list] should exist and include information about the datum in order to use this program.
- 6.5.3 DW-HYDRO Displays the same information as 6.5.1, in the form of a hydrograph (A4 size). The y-axis can have the

values increasing up the page or it can be inverted (values decreasing). There is a choice of plotting the data: (i) the points only, (ii) the points joined by straight line segments, (iii) the points joined by a smooth curve (a cubic spline).

6.5.4 WL-HYDRO

Displays the water levels above mean sea level (c.f. 6.5.2) in the form of a hydrograph. The same options are available as for 6.5.3.

6.5.5 WL-DIFSUM

Using the [Water-level] data, estimates the water levels at specified regularly spaced dates and produces for each time period a summary of the change in the water level at each grid reference.

6.5.6 WL-DIFMAP

Displays the same information as 6.5.5, plotted on maps showing the relative positions of the wells and the values of the changes in water level.

6.6 Conductivity data

6.6.1 COND-SUMMARY

Produces for each grid reference a summary of the [Conductivity] data.

6.7 Temperature data

6.7.1 TEMP-SUMMARY

Produces for each grid reference a summary of the [Temperature] data.

6.8 Conductivity log data

6.8.1 LOG-CONDSUM Produces for each grid reference a summary of the
 [Log-cond] data.

6.9 Temperature log data

6.9.1 LOG-TEMPSUM Produces for each grid reference a summary of the
 [Log-temp] data.

6.10 Keyfile

6.10.1 KEY-SUMMARY Produces a summary of the information which is
 currently stored on the Keyfile.

APPENDIX A - Index of control words

ADD-CODE

Adds code details to the system (for user-defined codewords).

Following by DATA-CARDS or DATA-FILE

ADD-FILE *filename*

Adds data to a file which already exists on the system

filename is the name of the data-type

Must be followed by DATA-CARDS or DATA-FILE

BAL-SUMMARY *lim 1, lim 2, ..., lim n/options*

Summaries of [Chemistry] samples for which balance falls in ranges: $\text{lim } 1 < |\text{balance}| < \text{lim } 2$

$\text{lim } (n-1) < |\text{balance}| < \text{lim } n$

options: either 'ALL' for both complete and

incomplete analyses or leave blank for complete analyses only.

Obviously, the chemistry quality control program (see QUALITY) must have been done previously, for calculation of balance.

If the standard list has not been included, (i.e. *options* is blank) then two cards with columns 1 to 8 blank; the information in columns 9 to 80 will be printed verbatim at the bottom of each summary (this can, for example, be used to explain the meanings attached to the asterisks). The end of the format cards must be indicated by an END card.

COND-SUMMARY Summary of the [Conductivity] data.

DATA-CARDS Indicates that data to be added to system follows punched cards.
Followed by ENDRUN, and then data cards.

DATA-FILE *Qualifier*filename (.elementname)*
Indicates that data to be added to system is in a mass storage file (or element).
Followed either by ENDRUN, or by END (in which case other manipulations of the data system may follow).

N.B. *elementname* is included only if the data is an element.

From *To*

DW-HYDRO From *start-date* to *end-date* options

Hydrographs showing depth to water table

Dates are in I6, e.g. 191173 for 19 November 1973; *start-date* in columns 18-23; *end-date* in columns 28-33.

Options start in column 34; four options are available:

/L for points joined by straight line segments

/S for points joined by cubic spline

/I to invert y-axis

/R = *value* to specify range of values to be plotted on y-axis.

The options can be used in any combination, except that /L and /R cannot both be specified at once. If neither /L nor /R are specified, the data points only will be plotted; if /R = *value* is left out, the program calculates the scale of the y-axis for each individual hydrograph, depending on the values to be plotted.

DW-SUMMARY

Summary of [Water-level] file

EDIT-FILE

*Date type/qual*filename*

Replaces data which has been written to *qual*filename* using LIST-FILE, and corrected using the editor; *qual*filename* is deleted afterwards.

EDIT-KEY

*qual*filename*

Replaces Keyfile data which has been written to *qual*filename* using LIST-KEY and corrected using the editor; *qual*filename* is deleted afterwards.

END

Signifies the end of the current block of operations.

ENDRUN

The last control card in any set; followed by data cards if putting on data using DATA-CARDS.

ENDSELECT

Ends the use of the selected station index (SELECT or MAPSELECT) and causes program to revert to using full station index.

It should be noted that this control card causes the heading (see HEADING, MAPSELECT and SELECT) to revert to the default of 'ALL THE DATA'.

HOLDRUN

*qual*filename*

Prevents the runstream which is generated from being executed. If *qual*filename* is specified, the runstream is stored in that file; otherwise the runstream will not be kept.

HEADING

heading

Can be used to change the heading (which appears on the output together with the study title as specified on the TITLE card). Default is 'ALL THE DATA'; maximum length is 24 characters. The heading can also be changed by use of the control words SELECT or MAPSELECT. Note that the heading used on any particular piece of output is the most recently specified one; also that ENDSELECT will cause the heading to revert to the default.

KEY-SUMMARY

Summary of current state of Keyfile.

LIST-FILE

*data-type/qual*filename*

Writes out data of a particular *data-type*, into *qual*filename*, for editing and replacing using EDIT-FILE.

N.B. (i) *qual*filename* must be an unassigned file.

(ii) the formats in which the data are written out are as on the standard data forms.

If *data-type* is a library file, no further information is required.

For [Site-list] data the program will automatically include those items which appear on the standard data forms; if there are any non-standard items on the file, these should be listed, one per card, as follows:

Item-name/format

where *Item-name* starts in column 1 and it not more than 8 characters; *format* is either 'I' for integer variables, an integer n between zero and 9 for real variables (n is the number of decimal places which will be included for that item) or 'A' for character variables.

The end of the list is signified by a card with 'END' in columns 1-3.

For [Chemistry] data, the program will automatically include the sample number; all other data which is required must be listed in the manner described above for non-standard items on the [Site-list]. The last card must once again be an END card.

LIST-KEY *qual*filename*

Lists contents of Keyfile into *qual*filename* (which must be an unassigned file) formatted as on the data forms; it can then be updated, and replaced using EDIT-KEY.

LITH-LOG

Lithological log plotting.

LOC-SUMMARY

Site location summary - grid reference, borehole reference and location (from [Site-list]).

See SITE-SUMMARY for other [Site-list] information.

LOG-CONDSUM

Summary of [Log-cond] data

LOG-TEMPSUM

Summary of [Log-temp] data

MAPSELECT *heading*

Selection of relevant stations prior to plotting maps - this automatically includes all [Boundary] data in the selection.

Followed by selection criteria (see Chapter 3) (N.B. only CODE and GRID criteria can be used in conjunction with MAPSELECT - the mapping programs automatically include only those grid references which appear within the map area). The selection criteria must be followed by an END card. *heading* will appear on the title block (maximum length is 24 characters).

See also HEADING and SELECT.

NEW-KEY

Replacement of Keyfile.

Must be followed by DATA-FILE or DATA-CARDS.

NEW-LIBRARY *data-type*

Opening a new library file.

Must be followed by DATA-CARDS or DATA-FILE.

NEW-MASTER *data-type*

Opening a new master file.

Must be followed by DATA-CARDS or DATA-FILE.

NEW-SYSTEM

Starting a new system; must be followed by
NEW-MASTER or NEW-LIBRARY.

OLD-FILE

data-type

Used to delete a particular *data-type* from
the system - must be followed by NEW-MASTER or
NEW-LIBRARY.

PEN

options

Used to specify pen size to be used in plotting
programs.

Options: BIRO - for biro plots

.3)
.4)
.5) for ink plots
.6)
.8)

Default (in no PEN card) is BIRO.

PIPER

size/balance %/options

Piper diagrams for [Chemistry] samples.

size: A4 or A3

balance: limit on balance - reject samples for
which balance exceeds this value.

options: COMPLETE ANALYSES (i.e. including only
those analyses which have determinations for
all the major ions).

ALL ANALYSES (i.e. including all
analyses with sufficient information to plot).

QUALITY

data type options

Quality control for standard data types.

data type can be: PUMPING-TEST

LITHOLOGY

LOG-TEMP

LOG-COND

WATER-LEVEL

CHEMISTRY

options: leave blank except for

- (i) [Water-level] - parameter δ in columns 25-34 in F10.0 format.
- (ii) [Chemistry] - ALL in columns 25-27 for all samples; blank for only those samples changed since last run of QUALITY for [Chemistry] data.

RATIO

: *ratio 1* : *ratio 2* : , ... , etc.

Summary of chemical ratios.

Each ratio should be separated by a colon; two colons to denote end of list (up to 6 ratios).

No blank spaces in list.

Each ratio 1, 2 ... n can take one of the

following forms: Item X/Item Y
Item Y
1/Item Y

where Item X, Item Y are the names of items on the [Chemistry] file.

The second form will simply give the value of Item Y, and the third form will give its reciprocal.

SELECT

heading

Selection of relevant stations.

Followed by selection criteria (see Chapter 3);
selection criteria must be followed by an END
card.

If plotting of maps is to be done, then MAPSELECT
must be used instead.

heading will appear on the title block (maximum
length is 24 characters.

See also HEADING.

SITE-SUMMARY

Summary of the [Site-list] data except for the
description location (see LOC-SUMMARY).

n is the number of screens to include on the
summary - it can take values 1, 2, 3 or 4 -
the default, if it is not specified, is number
which are stored on the data system.

Additional non-standard items can be included
in the summary by including format cards, one per
item:

Columns 1 to 8 - item name as stored on the data
system.

Columns 9 to 18 - format in which this item is
to be written ('6X, A4' for character variables
'I10' for integer variables
F10.x, where *n* is the number of
decimal places, for real
variables)

Columns 19 and 20 - a slash '/' in either of these
columns will result in a blank line following
this item. (cont)

Columns 21 to 32 - the name by which this
item will be identified on the summary.
Followed always (even if no additional items)
by END card.

SITEMAP

Map showing relative positions of sites,
together with their well reference number.

Followed by a map description card:

Columns 1 to 6 'ORIGIN'

Columns 9 to 16 : grid reference of bottom
left-hand corner of map.

Columns 17 to 22 : '/SCALE' - or '/XMAX'.

Columns 24 to 31 : either scale of map (in
grid units per centimetre) or maximum
X-value to be plotted on map - F8.0 format.

Columns 32 to 36 : '/GRID'

Columns 38 to 40 : interval between grid lines,
in grid units (I3 format).

Columns 41 to 45 : either '/A4', or '/A3' or
'/SIZE'.

Columns 47 to 51 : if '/SIZE', length of map
in centimetres.

Columns 52 to 56 : if '/SIZE', height of map
in centimetres.

Followed by one card, either 'BOUNDARIES' or
'NO BOUNDARIES'.

STIFF *balance %/options*

Stiff pattern diagrams for all samples for which the balance is less than *balance*.

options : 'COMPLETE ANALYSES' (i.e. including only those analyses which have determinations for all the major ions).

'ALL ANALYSES' (i.e. including both complete and incomplete analyses).

TEMP-SUMMARY

Summary of the [Temperature] data

TEST-PLOT *options*

TEST-SUMMARY

Line-printer summaries of pumping tests.

TITLE *study title*

The first card in any run.

study title is a descriptive title (< 24 characters) which appear at the top of all the output as part of the title block.

WL-DIFMAP

options

Water level differences estimated at specified intervals and plotted on a map.

options: 'INTERVAL' in columns 13-20

length of interval (I4 format) in columns 21-24 'DAYS', 'MONTHS', or 'YEARS', starting in column 26.

'FROM' in columns 34-37.

Start date (E.G. 171273 - 17 December 1973) in columns 39-44.

either ('TO' in columns 46-47
(end date in columns 49-54

or (number of dates of which estimates
(required (I4 format) in columns 46-49
('DATES' in columns 51-55.

Followed by a map description card, and a card with 'BOUNDARIES' or 'NO BOUNDARIES' exactly as described under SITEMAP.

WL-DIFSUM

options

Line printer summary of water level differences estimated at specified intervals.

options: exactly as described above under WL-DIFMAP.

WL-HYDRO

FROM *start date* TO *end date options*

Hydrographs showing water levels above mean sea level. This program uses the [Water-level] file and the datums from the [Site-list] ; obviously it can only be used if the datums have been recorded. The exact format of the card is as described for DW-HYDRO.

WL-SUMMARY

Summary of water levels above mean sea level, using the [Water-level] file and the datums from the [Site-list].

APPENDIX B - Error messages

Errors in the input to the program CONTROL are indicated by a message 'DIAGNOSTIC x', where x is an integer. In addition the program lists the control cards which had been read in before the error was detected, and the runstream which was generated (see Table 1 - Control Program Status). Since each card is read in and processed in turn, the error will usually be on the last card which was read in; the list below, of diagnostic messages and the meanings attached to them, should help to further pinpoint the source of the error.

DIAGNOSTICS

TITLE card missing
or TITLE card is present, but the project title has been left
blank.

a NEW-SYSTEM card has been included, but it is not followed
by either NEW-LIBRARY or NEW-MASTER.

attempting to add data, but no DATA-FILE or DATA-CARDS to
indicate location of the data.

SYSTEM ERROR.

unrecognisable control word.

SYSTEM ERROR.

using a forbidden filename (e.g. attempting to change system-
defined files).

no END or ENDRUN card where one was expected.

SYSTEM ERROR.

attempting to make too many selections.

10 mapping program (SITEMAP or WL-DIFMAP) but plotting details are
absent or badly defined.

11 mapping program - cannot ask for boundary plotting after using
SELECT to make a selection (must use MAPSELECT).

error on LIST-FILE or EDIT-FILE card.

TESTPLOT- need to specify 'LOG-LOG', 'LOG-LIN', or 'BOTH' in
columns 13-19, depending on type of plot required.

14 QUALITY with incorrect filename (i.e. one for which there is
no quality control program).

15 attempting to use MAPSELECT with either 'BOX' or 'QUAD' selection
criteria - should only use 'CODE' or 'GRID'.

16 name of data type has been omitted.

OLD-FILE following NEW-SYSTEM.

18 ADD-FILE following OLD-FILE (should be followed by NEW-LIBRARY
or NEW-MASTER).

19 mapping program, but have not specified either 'BOUNDARY' or
'NO BOUNDARIES'.

20 QUALITY for 'WATER-LEVEL' and 'CHEMISTRY' requires additional
data on control card.

21 asking for a map which will not fit on 36" paper.

- 22 error on WL-HYDRO or DW-HYDRO card.

- 23 the pen size specified on the PEN card is not available
(should be .3, .4, .5, .6 or .8).

- 24 error on PIPER card.

- 25 error on STIFF card.

- 26 error on RATIO card

- 27 error on BAL-SUMMARY card.

- 28 error on CHEM-SUMMARY card.

APPENDIX C - Miscellaneous Points

1. Units

For data of standard types (see table 2) the units to be used are specified in "Using the Groundwater Data Forms". However, in the case of [Chemistry] data which has been coded up in mg/l, conversions to meq/l will be performed as follows:

Determination	Abbreviation	Conversion factor
Calcium	CA	.0499
Magnesium	MG	.08224
Sodium	NA	.0435
Potassium	K	.02558
Carbonate	CO3	.03333
Bicarbonate	HCO3	.01639
Hydroxide	OH	.0588
Sulphate	SO4	.02082
Chloride	CL	.0282
Nitrate	NO3	.01613
Nitrite	NO2	.02174

All subsequent operations on the data will then be performed using the new units.

N.B. Other conversions can be performed only after additional programming.

@RUN WHM, 33-24, SAFI

@SETC 6

@XQT ODM * CONTROL . CONTROL

TITLE_ _ _ _ _ SAFI

NEW-SYSTEM

NEW-LIBRARY_ WATER-LEVEL

DATA-FILE_ _ _ HMOREL * SAFI. WATER-LEVEL

END

NEW-MASTER_ _ SITE-LIST

DATA-FILE_ _ _ HMOREL * SAFI. INVENTORY

ENDRUN

@XQT ODM * CONTROL CONTROL

TITLE_ _ _ _ _ SAFI

WL-SUMMARY

LOC-SUMMARY

ENDRUN

@XQT ODM * CONTROL . CONTROL

TITLE_ _ _ _ _ SAFI

WL-HYDRO_ _ _ _ _ | _ _ _ _ _ 0104.77_ _ _ _ _ 010480/I/R = 1.999

WL-HYDRO_ _ _ _ _ FROM_ _ 010477_ _ TO_ _ 010181