QADATA USER'S MANUAL: AN INTERACTIVE COMPUTER PROGRAM FOR THE RETRIEVAL AND ANALYSIS OF THE RESULTS FROM THE EXTERNAL BLIND SAMPLE QUALITY-ASSURANCE PROJECT OF THE U.S. GEOLOGICAL SURVEY

By Keith J. Lucey

U.S. GEOLOGICAL SURVEY

Open-File Report 90-162

Denver, Colorado
1990

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ABSTRACT

The U.S. Geological Survey conducts an external blind sample quality-assurance project for its water-analysis laboratories in Denver, Colorado, and Ocala, Florida, based on the analysis of reference water samples. Reference samples containing selected inorganic and nutrient constituents are disguised as environmental samples and are sent periodically through Survey offices to each laboratory. The results of this blind sample project indicate the quality of analytical data produced by the laboratories.

This report provides instructions for the use of QADATA, an interactive, menu-driven program that allows data users to retrieve the results of the blind sample quality-assurance project. The QADATA program, which is available through the U.S. Geological Survey's national computer network, accesses a blind sample data base that contains more than 50,000 determinations from the last five water years for approximately 40 constituents at various concentrations.

The data can be retrieved from the database for any user-defined time period and for any or all available constituents. After the user defines the retrieval parameters, the program prepares statistical tables, control charts, and precision plots and generates a report which can be transferred to the user's office through the computer network. A discussion of the interpretation of the program output is also included in this report.

This quality-assurance information will permit users to document the quality of the analytical results received from the laboratories. The blind sample data is entered into the database within weeks after being produced by the laboratories and can be retrieved to meet the needs of specific projects or programs.

INTRODUCTION

The National Water-Quality Laboratory (NWQL) of the U.S. Geological Survey, located in Denver, Colorado, and the Survey's Water Quality Services Unit (WQSU), located in Ocala, Florida, routinely analyze water samples for inorganic and nutrient constituents and physical properties (Fishman and Friedman, 1989). Annual summaries of the external blind sample quality-assurance project used to monitor the quality of the work at the NWQL provide a detailed description of the project (Peart and Thomas, 1983a, 1983b, 1984; Peart and Sutphin, 1987; Lucey and Peart, 1988, 1989a, 1989b; Lucey, 1989). Beginning in water-year 1990, an external blind sample quality-assurance project was implemented for the WQSU similar to the one used at the NWQL.

This report provides instructions for the use of QADATA, an interactive, menu-driven computer program that allows data users to access an on-line data base containing the results of the blind sample quality-assurance program. This data base, which is available through the U.S. Geological Survey's national computer network, contains more than 50,000 blind sample values for inorganic and nutrient constituents determined by several analytical methods at various concentrations. Data from dilute precipitation samples analyzed by the low-ionic strength section of the NWQL also are included in this data base.

The data can be retrieved from the data base for any user-specified time period and for any or all available constituents. After the user defines the retrieval, the program generates a report containing statistical tables, control charts, and precision plots of the retrieved data. A discussion of the interpretation of the program output is also included.

BLIND SAMPLE PROJECT DESCRIPTION

The blind sample quality-assurance project is based on the analysis of reference water samples. Standard reference water samples (SRWS) are prepared from natural waters spiked with selected analytes. The SRWS are sent through a round robin interlaboratory testing program from which a most probable value (MPV) is determined for the concentration of each constituent (Skougstad and Fishman, 1975; Schroder and others, 1980; Janzer, 1985).

The Survey's Water Quality Services Unit in Ocala, Florida prepares blind reference samples by diluting the SRWS with deionized water, mixing two SRWS in varying proportions, or using the SRWS undiluted. The MPV of each constituent in the sample is calculated from the known percentage of each SRWS in the mixture. This preparation allows a larger number of unique reference samples to be available for use in the blind sample project with varying concentrations of analytes. The reference samples are then disguised as environmental samples and sent periodically through other Survey offices to each laboratory for analysis.

Quality-assurance data from the blind sample project are retrieved from the laboratories on a weekly basis and analyzed for precision and accuracy. A report is prepared for laboratory personnel each week containing control charts that illustrate quality-assurance data for inorganic and nutrient constituents from various analytical methods. In addition, a monthly statistical report containing precision and accuracy data, which indicates the quality of data produced by the laboratory during the previous five-month period, is supplied to district quality-assurance personnel.

After being retrieved from the laboratories, blind sample data are stored in the Survey's National Water Data Storage and Retrieval System (WATSTORE). This data is then downloaded to a separate data base containing only blind sample quality-assurance data, which is maintained on a node (QVARSA) of the Survey's national computer network. The blind sample data is entered into this data base within weeks after being produced by the laboratories.

INTERACTIVE RETRIEVAL AND ANALYSIS OF QUALITY-ASSURANCE DATA

QADATA is an interactive, menu-driven program that allows users to retrieve the results from the blind sample quality-assurance data base for any user-defined time period and for any or all available constituents in order to meet the needs of specific projects or programs. Appendix I provides a listing of all constituents available in the data base from the NWQL for four types of data (major ions, trace metals, nutrients, and precipitation). Appenix II provides a listing of constituents for the Ocala WQSU, where low-ionic strength (precipitation) data and inductively coupled plasma emission spectrometry (icp) data are not available.

After the user defines the retrieval, the program generates a report containing statistical tables, control charts, and precision plots which can be transferred to the user's office through the computer network or displayed on the user's terminal screen. The report file is sent through the computer network to the fts_depot at the node designated by the user, where it can be printed at the site's line printer in 132-column format.

The QADATA program is maintained on QVARSA at the Survey's headquarters in Reston, Virginia, and consists of several separate computer programs. A brief summary of these programs and their relationship follows:

1. USER.CPL (Appendix III): A command procedure language (CPL) file that begins interactive dialogue and accesses the blind sample data base.

2. QAMENU.PGM (Appendix IV): An INFO1 program, invoked from within the CPL, that allows interactive input to access the blind sample data base and define retrieval specifications.

3. QA1.TRANS (Appendix V): A P-STAT1 program, called if the user chooses to have the statistical report output to the terminal screen as an interactive session, that generates statistical tables and charts and accepts keyboard input to scroll through the report.

4. QA.TRANS (Appendix VI): A P-STAT program, called if the user chooses to have the statistical report transferred through the computer network, that generates tables and charts and incorporates them into a final report.

5. USERPH.CPL (Appendix VII): A CPL to submit the QA.TRANS program, which runs in phantom mode at a low priority on the computer system to minimize demand on computer resources during statistical analysis and report generation, reducing its effect on response times of other users on the system.

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1. Use of trade names in this report are for identification purposes only and does not constitute endorsement by the U.S. Geological Survey

An example retrieval session using the QADATA program is presented to illustrate the various commands required to operate the program and instruct the reader on their use. Although QADATA is a menu-driven, user-friendly program and each step in the process is documented for the user on the terminal screen, this instructional report is meant to complement the on-line documentation so the user can be familiarized with the responses required for the various prompts in preparation for a retrieval session.

In this example, blind sample quality-assurance data for dissolved solids during calendar year 1986 is retrieved for the National Water-Quality Laboratory and the final statistical report is output to a computer file. Underlined text in bold letters indicates interactive input by the user from the keyboard; lower case indicates text displayed on the screen; the character string '....' indicates text has been left out in the interest of brevity; the symbol '<CR>' represents a carriage return; numerals in parentheses refer to numeric order for terminal screen displays from the program (ie. (1) represents the first screen display that a user would see after invoking the program); and a brief explanation precedes each screen display enclosed in brackets (ie. [...]) next to its numeral.

Instructions to Access the QADATA Program

To invoke the QADATA program, the user logs into QVARSA and enters the command 'QADATA':

NETLINK -TO QVARSA <CR>
PRIMENET....
LOGIN (your userid) <CR>
Password? (your password) <CR>

....

OK, QADATA <CR>

Only one user is allowed to use the QADATA program at a time. If you try to invoke the program when a retrieval is in progress, access will be denied; you will be requested to try again later and you will then be returned to your origin directory on QVARSA. Invoking the program ten to fifteen minutes later should result in successful access.

Instructions for Input to Define a Retrieval

Following are examples of the terminal screen output from the QADATA program with instructions for interactive input:

(1) [Entries to these two prompts are required to properly tag data files and provide a destination for the final statistical report.]

```
WELCOME TO THE BLIND SAMPLE INTERACTIVE RETRIEVAL PROGRAM
**********************************************************
USERID:      needed to tag data files.
PRIME NODE: needed as a destination for output data file.
**********************************************************

Enter your userid: (your userid) <CR>

Enter your PRIME node: (your PRIME node) <CR>
```

(2) [The user simply needs to read this screen, be sure the keyboard is in the 'CAPS LOCK' mode, and enter a carriage return <CR> to continue.]

```
                    BRANCH OF QUALITY ASSURANCE

                    DATA BASE FOR BLIND SAMPLE PROJECT

**********************************************************************

This program allows you to access the blind sample quality-assurance
data base for the National Water Quality Laboratory and the data base
for the laboratory of the Water Quality Services Unit in Ocala for any
or all of several inorganic constituents (major ions, trace metals,
nutrients, and low-level concentration precipitation samples) for any
time period that you define.

Control charts, precision plots, and several statistical tables will be
generated, which will indicate the quality of the analytical data
produced by the laboratory during the time period that you request.

The program will prompt for the necessary information.  Please be sure
your keyboard is in the "CAPS LOCK" mode.

              (hit "return" or enter any key to continue)  <CR>
```

(3) [The user can choose to access the QA data base for the NWQL or Ocala WQSU by entering <CR> or '33', respectively, or exit the program by entering '99'. QA data for only one laboratory at a time can be retrieved during a single terminal session.]

....

BE SURE YOUR KEYBOARD IS IN THE "CAPS LOCK" MODE
(Retrieve data for only one laboratory per login session)

Then choose one of the following: <CR>

Enter any key or "return" = access NWQL QA data base
Enter 33 = access Ocala WQSU data base
Enter 99 = no more retrievals, exit program

(4) [In this step the user begins to define the QA retrieval by choosing a data type. The program accesses only one data type at a time, but after a retrieval has been completed (for major ions in this example), the program will allow the user to return to this screen and access another data type. All four data types can be retrieved during a single session with four passes through the program to define the retrieval. Two different retrieval sessions are necessary if the user wants to analyze data from two different time periods for the same data type.]

QUALITY-ASSURANCE DATA BASE FOR ROUTINE WATER-ANALYSES

What type of QA data would you like to access?
(there is no precipitation data for the Ocala WQSU)

M = MAJOR IONS
T = TRACE METALS
N = NUTRIENTS
P = PRECIPITATION (LIS)

Select one type or "99" to exit program M <CR>

(5) [The beginning and ending dates to define the retrieval are now entered (calendar year 1986 in this example). The quality-assurance samples are retrieved by the dates the samples were logged into the laboratory. Beginning date must be less than ending date in the 'yyyymmdd' format shown on the screen. The most recent data available would be within one to two months - this is due to a time lag between the login of the sample, the release of the analysis by the lab, and review of values before updating the blind sample data base.]

AVAILABILITY OF QUALITY-ASSURANCE DATA TYPES

	NWQL	WQSU
MAJORS	1985 - present	1989 - present
TRACE METALS	1985 - present	1989 - present
NUTRIENTS	1986 - present	1989 - present
PRECIPS	1986 - present	

(most current data is 1 - 2 months prior to the present)

Enter the beginning and ending login dates for your period of interest using the yyyymmdd format (ie. 19881019 = October 19, 1988).

Beginning date: 19860101 <CR>

Ending date: 19861231 <CR>

(6) [The number of records selected is shown on the terminal screen for two seconds. No interactive input is required. Invalid dates or entries in the previous step would results in 0 records being selected. In the case of a null retreival the user should simply finish the retrieval by following screen prompts, which will eventually bring up screen (3) where a new retrieval session can be started.]

4382 RECORDS SELECTED

(7) [A list of constituents for the chosen data type appears on the screen. In some cases data is available for more than one analytical method (ie. calcium by atomic absorption spectrometry - CAAA, and by inductively coupled plasma emission spectrometry - CA). Enter only one at a time; the program will also cycle through this step so the user can choose additional constituents. By entering 'ALL', data for all listed constituents can be retrieved in one entry rather than cycling through the process entering constituents individually. Dissolved solids (ROE) has been chosen in this example.]

CHOOSE THE "ALL" OPTION TO RETRIEVE DATA FOR ALL MAJOR CONSTITUENTS.
YOU CAN CHOOSE CONSTITUENTS INDIVIDUALLY USING THE INDICATED PROMPT.
(all constituents in dissolved phase)

(icp = inductively coupled emission spectrometry)
(aa = atomic absorption spectrometry)

ALK - alkalinity	B - boron
CA - calcium icp	CAAA - calcium aa
CL - chloride	ROE - dissolved solids (at 180° C)
F - fluoride	MG - magnesium icp
MGAA - magnesium aa	K - potassium
SIO2 - silica icp	SICOL - silica, colorimetry
NA - sodium icp	NAAA - sodium aa
SO4 - sulfate	ALL - retrieve all major constituents

Choose only one: (return to end) ROE <CR>

(8) [As the program searches the data base for the appropriate QA data, a screen display appears indicating that there could be several seconds of computational time. No interactive input is required.]

This step sometimes takes several seconds

(9) [After the retrieval for each constituent is completed, this screen appears and indicates the number of records retrieved. No interactive input is required.]

THIS PORTION OF YOUR RETRIEVAL IS 416 RECORDS:
This step may take a few seconds - wait for the next prompt

(10) [By entering '1' the user is returned to the previous list of constituents for the data type of interest (screen 7). The user can cycle through the list of constituents as many times as necessary with an affirmative response in this step. An entry of '2' terminates the retrieval for the data type. In this example only data for dissolved solids from the list of major ions is retrieved.]

Do you want to retrieve more majors for this period? 2 <CR>
1 = yes, 2 = no

(11) [This screen results from a negative response in (10). A carriage return is entered.]

You have finished your retireval of this range of QA data. You will now be returned to the initial program setup where you can either continue retrieving data from the other types of QA data or leave the retrieval portion of the program.

ONLY RETRIEVE DATA FOR ONE LABORATORY PER TERMINAL SESSION

(hit "return" or enter any key to continue) <CR>

(12) [At the program set-up screen, the user can begin a new retrieval session for another data type by entering a carriage return or terminate the retrieval portion of the program by entering '99'. Data from retrievals for additional data types is appended to the previous data until the program is terminated.]

BE SURE YOUR KEYBOARD IS IN THE "CAPS LOCK" MODE

Then choose one of the following: 99 <CR>

Enter any key or "return" = access NWQL QA data base
Enter 33 = access Ocala WQSU QA data base
Enter 99 = no more retrievals, exit program

(13) [This screen appears after exiting the retrieval portion of the QADATA program. A carriage return is entered by the user.]

A file of the data that you have retrieved will be saved in our USER.DIR as "(your userid).QADATA.(date).(time)" for one week. This file contains the raw QA data and you can request a copy from the Blind Sample Project.

The program will now prepare control and precision charts for your data. You can choose to have the final data report displayed at your terminal screen or transferred to your PRIME as "FTS_DEPOT>QAPLOTS.(your userid).(date).(time)".

PLEASE NOTE: OUTPUT TO THE SCREEN SHOULD ONLY BE USED FOR RETRIEVALS OF ONE OR TWO CONSTITUENTS

(hit "return" or enter any key to continue) <CR>

(14) [Before invoking the P-STAT statistical software, the user has to choose the method of outputting the final statistical report. The screen is self-explanatory and in this example the 'NO' entry calls the phantom CPL to generate the report. Finally, the user indicates whether data was retrieved from the Ocala WQSU so the program can tag the final report with the proper laboratory name.]

****
YOUR DATASET IS READY TO ENTER THE PLOT PORTION OF THE PROGRAM
****
At the next prompt, please answer "YES" or "NO":

YES = plots and tables are output to the terminal screen in 80-column format. PLEASE DO NOT USE THIS OPTION IF YOUR RETRIEVAL CONTAINS MORE THAN TWO CONSTITUENTS! This option is only recommended for small retrievals since large datasets can affect response time for other users on the system. Your terminal will remain in interactive mode and will require keyboard input for several prompts during the session. Plots and tables are NOT output to a file on the PRIME.

NO = plots and tables are NOT output to the screen but are output to a plot file in 132-column format and transferred to the fts_depot at your PRIME. A system phantom finishes the program without interactive input.
****

DO YOU WANT TO VIEW PLOTS ON YOUR TERMINAL SCREEN? NO <CR>

PLEASE ANSWER YES OR NO TO THE NEXT PROMPT.

DID YOU RETRIEVE DATA FOR THE OCALA WQSU? NO <CR>

(15) [In the final step of the process the user is informed that the phantom has been invoked and of the computer file name for the statistical report. The final report is usually transferred within the hour to the computer node designated by the user in screen (1). Finally, the user is returned to the origin directory on QVARSA.]

```
....

PHANTOM is user 144
**************************************************************
A system phantom will now generate a final file of your dataset
and transfer it to your fts_depot as QAPLOTS.your userid.date.time
....
**************************************************************
*         Your session in the BQA data base is finished        *
**************************************************************
OK, LO <CR>
```

Explanation of Statistical Output

The statistical report generated by the QADATA program includes statistical tables, control charts, and precision plots. The report is either displayed on the terminal screen or placed in a computer file and transferred to the user's office through the computer network. In this section an explanation of the output contained in the report that was generated by the preceding retrieval of dissolved solids data for calendar year 1986 is presented. An example of a final report displayed on the terminal screen is presented in the following section. Although only one constituent is used in this example, all listed constituents for all four data types could be contained in a single report.

Factors that need to be considered for interpretation of the results from the QADATA program include the following:

1. No effort is made to correct nonanalytical errors, even when it is obvious which corrective measures are appropriate, so the data are preserved as produced by the laboratory. These errors include any made in logging the sample into the laboratory and data entry errors. Errors of this type detected by data reviewers in Survey offices may improve data quality when compared to that inferred from the QADATA statistical report.

2. No quality-assurance samples had any constituents redetermined except those requested by the laboratory internal quality-control groups. Requests for reanalysis by data reviewers in Survey offices may result in the detection of analytical and nonanalytical errors, improving data quality when compared to that inferred from the QADATA statistical report.

3. Control charts generated by QADATA may be used to determine analytical conditions at any given time period. In some situations, statistical tests indicate that an analytical process is in control for a certain time period but closer examination of the data reveals that the process is out of control for a short portion of this time period. Data interpretation can be improved by using the QADATA program to define the period in question and determine the precision and accuracy of the analytical method for the shorter time period.

4. Several data points may seem to be in error because of an incorrectly applied dilution factor. Sample dilutions are made routinely in the laboratory to bring sample concentrations into analytical range. If the dilution factor is not applied or is applied incorrectly, the reported value will be in error by the amount of the dilution factor. These kinds of errors are difficult to confirm. Their detection, confirmation through rerun requests, and correction in the field offices will increase the reliability of the data above that indicated by the program.

5. Non-analytical errors for nutrient determinations can result when the samples are not maintained at the ideal temperature of 4^{o} C during shipping and receiving.

Most probable standard deviations (MPSD) are determined by using linear least squares equations developed by regressing the means of each constituent obtained from all the SRWS analyzed during the last eight years against the corresponding standard deviations for the constituent. These regression equations are updated at the beginning of each water year by including the data from SRWS prepared during the previous year. This method enabled an estimation of a MPSD for each constituent on a sample-by-sample basis to ascertain whether the determination in question was statistically in or out of control. Number of standard deviations (NSD) plotted on control charts is calculated:

$$NSD = (\text{Reported value} - MPV) / MPSD$$

where reported value refers to the value reported by the laboratory, MPV is most probable value, and MPSD is the most probable standard deviation.

The number of determinations for each constituent in the retrieval, the number of these that are outside the control limits of two standard deviations from the MPV, the number more than six standard deviations from the MPV, and the percentages of each are provided by the program as shown in Table 1. Results that are more than six standard deviations from the theoretical value are considered outliers and are usually either the result of a bottle mix-up when the sample is logged into the laboratory or transcription errors of the analytical results. In the dissolved solids data for 1986, 27 out of 416 determinations, or 6.5 percent, are outside the statistical control limits and 2 of the 27 are greater than six standard deviations from the MPV. Applying binomial-probability-distribution equations to the data using procedures described by Friedman, Bradford, and Peart (1983), and by Peart and Thomas (1983a), it can be determined that the analytical method is within statistical control at the 95 percent confidence level for calendar year 1986.

TABLE 1: CONSTITUENTS IN RETRIEVAL WITH NUMBER OF DETERMINATIONS
****

TYP = data type, M=major, T=trace metal, N=nutrient, P=precip
TOT.NUM = total number of determinations
NUM.2SD = number more than 2 standard deviations from theoretical
NUM.6SD = number more than 6 standard deviations from theoretical
PERCENT.OVER.2SD = percent more than 2 std dev from theoretical
PERCENT.OVER.6SD = percent more than 6 std dev from theoretical

TYP	ION	TOT NUM	NUM SD2	NUM SD6	PERCENT OVER. 2SD	PERCENT OVER. 6SD
M	ROE	416	27	2	6.5	0.5

The range of theoretical concentrations (most probable values or MPV's) present in the retrieved data set are shown as Table 2. This information allows a user to scrutinize the ranges represented and determine comparability to those in the project data set of interest. The range of the dissolved solids QA data is 35 to 1106 milligrams per liter (mg/L).

TABLE 2: RANGE OF THEORETICAL CONCENTRATIONS (MPV) BY CONSTITUENT
****

TYP = data type: M=major, T=trace metal, N=nutrient, P=precip
High and Low values reported in milligrams per liter, except for trace metals (T) and boron (B) which are in micrograms per liter.

TYP	ION	Low	High
M	ROE	35	1106

Control charts (fig. 1) are output with the number of standard deviations (NSD) from the theoretical value plotted against the date the sample was logged into the laboratory. The DECIMAL.DATE format for login date values represents a fraction of a month (ie. 4 = April 1; 4.5 = April 15; etc.). If the reported value is within two standard deviations of the theoretical value it is considered within statistical control. The plot is annotated in the upper left-hand corner by data type (TYP = M), the constituent or ion (ION = ROE), and the year (YEAR = 1986).

Even though the statistical tests applied in Table 1 indicate the analytical method is within statistical control for the year, the appearance of the control chart for dissolved solids data for 1986 (fig. 1) suggests that data from the period September 1 through November 1 may be suspect. Most of the determinations from the remainder of the year are within the two standard deviation control limit.

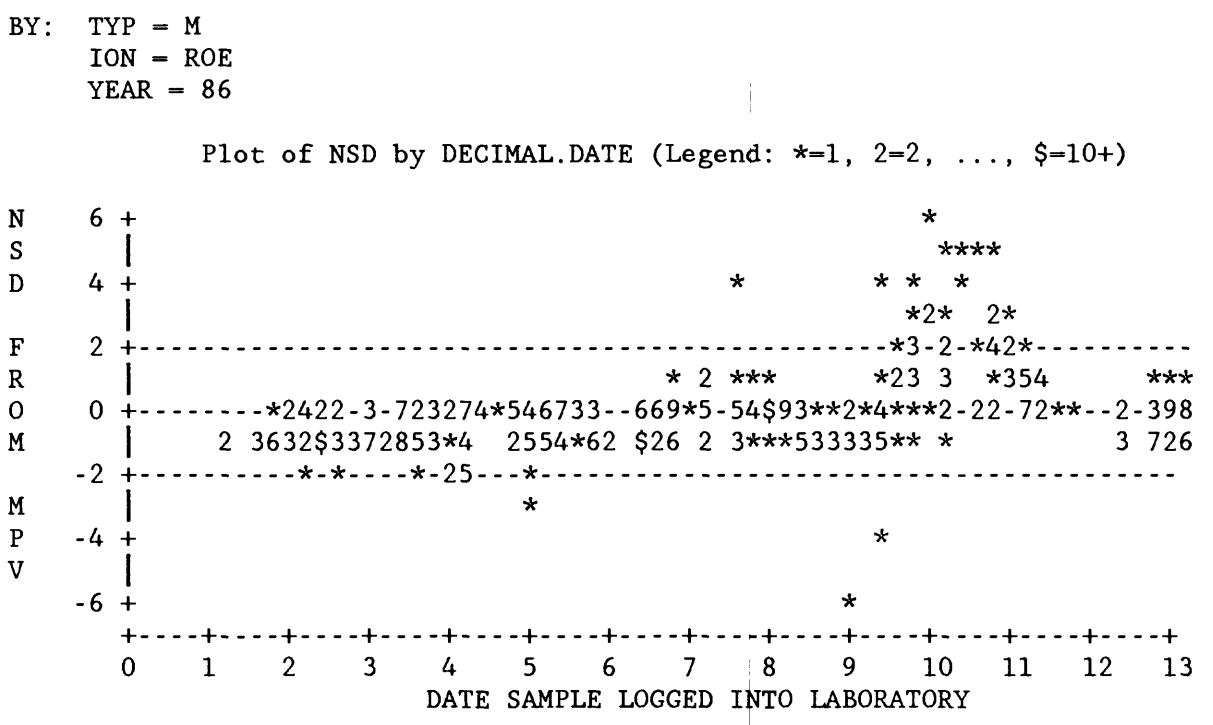

Figure 1: Control chart for dissolved solids, 1986, as output by the QADATA program.

Table 3 lists precision data used to calculate the relative standard deviation (RSD) for each mix represented in the data set by data type and constituent. Reading the first line of the table, there are six determinations (NUM) for dissolved solids of a mix with an MPV of 35.0 mg/L (MPV MIX); the mean of the values reported by the laboratory is 34.50 mg/L; the standard deviation (S.D.) of these values is 2.88; and the RSD is 8.35 percent. The RSD represents a percentage error at a given concentration and is calculated:

$$RSD = (S.D./Mean) * 100$$

The expected error for the determination of dissolved solids at a concentration of 35 mg/L is 8.35 percent. An indication of method bias can be determined by comparing the mean of the reported values with the MPV of the mix. There does not appear to be a strong indication of either positive or negative bias in this data set. Values that are more than six standard deviations from the MPV are removed from the data set and only those mixes with three determinations or greater are represented. As a result, although the range of MPV's in Table 2 indicate representation to 1106 mg/L, the highest MPV listed in the precision table is 975 mg/L.

TABLE 3: PRECISION DATA BY DATA TYPE AND CONSTITUENT

****

NUM (number of determinations) for each ION and TYP by unique mix; MPV.MIX is theoretical value for the unique mix, with the MEAN; S.D. (standard deviation); and the RSD (relative standard deviation, in percent) of the values reported by the laboratory. Values more than six standard deviations from theoretical are deleted.

TYP	ION	MPV MIX	NUM	Mean	S.D.	RSD
M	ROE	35.0	6	34.50	2.88	8.35
M	ROE	65.7	10	76.40	7.53	9.86
M	ROE	74.4	8	79.87	5.06	6.33
M	ROE	87.6	16	100.31	14.22	14.17
M	ROE	107.0	8	102.50	6.19	6.04
M	ROE	161.0	11	151.73	5.39	3.55
M	ROE	174.0	19	171.42	3.22	1.88
M	ROE	192.0	19	190.42	3.66	1.92
M	ROE	215.0	34	202.41	4.42	2.18
M	ROE	307.0	21	294.48	6.63	2.25
M	ROE	371.0	12	365.75	21.26	5.81
M	ROE	365.0	18	373.33	30.95	8.29
M	ROE	449.0	8	433.37	8.14	1.88
M	ROE	527.0	26	536.00	24.04	4.49
M	ROE	555.0	22	556.05	35.25	6.34
M	ROE	660.0	18	653.39	15.80	2.42
M	ROE	714.0	14	732.79	50.99	6.96
M	ROE	830.0	7	809.14	8.86	1.09
M	ROE	975.0	7	973.00	6.19	0.64
....						

Finally, the precision data is presented on precision plots with RSD on the y-axis and the mean of the reported values on the x-axis (fig. 2). The user can fit a trend line to the data and read an expected error for concentrations that were not represented in the retrieved data set or even extend a trend line to higher or lower concentrations on the plot to estimate an expected error.

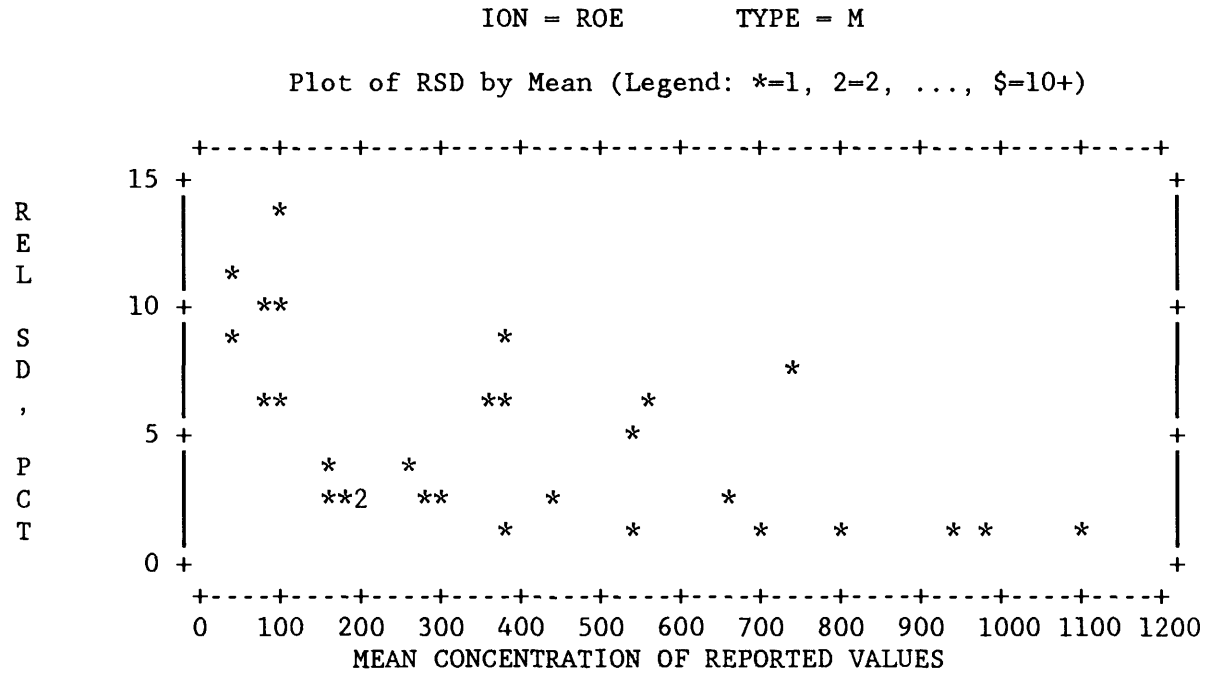

Figure 2: Precision data for dissolved solids, 1986, as output by the QADATA program.

Statistical Report Displayed on the Terminal Screen

Steps (1) - (13) are identical whether the final report is sent to the user through the computer network or displayed on the terminal screen in interactive mode. A response of 'YES' to the prompt in step (14) would result in the statistical report being displayed on the terminal screen. Since the phantom is not being invoked to generate a computer file report, step (15) is skipped with this option. In this next example, dissolved solids QA data has been retrieved for the time period September 1, 1986 - November 1, 1986. To view the final report the user has to be available at the keyboard to enter a carriage return to continue scrolling output. The program prompts for a response with 'HOLDING . ' A terminal with a 'print screen' option could be used to get hardcopy of the data contained in the report.

(16) [Comment lines in the P-STAT programming language indicate completion of various steps in the statistical process. A carriage return is entered to refresh the screen after the 'HOLDING . ' prompt and allow the program to continue its output.]

```
*** Your dataset is being loaded into the plot program ***
*** computing decimal date for control charts ***
     *** (ie. 3.5 = Mar 15; 4 = Apr 1;) ***

* CONTROL CHARTS WILL FOLLOW - PLEASE NOTE THESE ABBREVIATIONS *
TYP = data type (M - majors, N - nutrients, P - precipitation samples, T
- trace metals);  NSD = number of standard deviations; MPV = most
probable value or theoretical value.  Date on x-axis is decimal.date,
ie. 1 = Jan 1, 6.5 = June 15, 11.7 = November 21

*** At "HOLDING.." hit <CR> to continue ***
HOLDING..<CR>
```

(17) [Control charts are displayed by constituent followed by a 'HOLDING .' prompt. The number of standard deviations from the most probable value are plotted against time with the two standard deviation control limit indicated.]

```
 BY:  TYP = M
      ION = ROE
      YEAR = 86

       Plot of NSD by DECIMAL.DATE (Legend: *=1, 2=2, ..., $=10+)

N   6 +                    *
S     |                  *     *   *  *
D   4 +    *          *          *
      |            *    *  *   *          2   *
F   2 +-------*----*2--------**--------*22----2---*-----------
R     |     * 2   *2         *2          *    *2   5
O   0 +-*2-2--*----*----*----2------2----2--------5**---------
M     | 3* 4  *    *          *
   -2 +-------------------------------------------------------
M     |
P  -4 +      *
V     |
   -6 +----------+----------+----------+----------+----------+-
      9         9.5         10        10.5         11        11.5
                     DATE SAMPLE LOGGED INTO LABORATORY
 HOLDING .<CR>
```

(18) [An explanation of the next statistical table to be displayed is provided followed by a prompt for input.]

*** computing data for precision plots ***

****

Preparing display of constituents with total number of obs (TOT.NUM), number more than 2 s.d. (NUM.2SD) from the MPV, and number more than 6 s.d. (NUM.6SD) from the MPV.

Values greater than 6 standard deviations from the theoretical will be deleted from the dataset before calculating percent relative standard deviation and plotting of precision data.

*** At "HOLDING.." hit <CR> to continue ***

****

HOLDING .<CR>

(19) [A table of the number of determinations for each constituent in the retrieval is displayed (as Table 1) with an explanation of abbreviations. The number of values outside the control limits are provided. Values greater than six standard deviations from the theoretical value are usually due to sample mix-ups or transcription errors rather than problems with the analytical method.]

```
CONSTITUENTS IN RETRIEVAL WITH NUMBER OF DETERMINATIONS
************************************************************
TYP = data type, M=major, T=trace metal, N=nutrient, P=precip
TOT.NUM = total number of determinations
NUM.2SD = number more than 2 standard deviations from theoretical
NUM.6SD = number more than 6 standard deviations from theoretical

                                    PERCENT  PERCENT
              TOT    NUM    NUM     OVER.    OVER.
TYP   ION     NUM    SD2    SD6       2SD      6SD

M     ROE      80     24      1        30      1.2

*** More computing ***
...
*** At "HOLDING.." hit <CR> to continue ***
HOLDING .<CR>
```

(20) [A table of the range of theoretical concentrations for each constituent in the retrieval is presented (as Table 2) to indicate how comparable the QA data will be to data in a particular project.]

```
     RANGE OF THEORETICAL CONCENTRATIONS (MPV) BY CONSTITUENT
****************************************************************
TYP = data type: M=majors, T=trace metals, N=nutrients, P=precips
HIGH and LOW values reported in milligrams per liter, except for
trace metals (T) and boron (B) which are in micrograms per liter.

TYP   ION      Low  High

M     ROE     65.7   714

HOLDING .<CR>
```

(21) [Precision data is provided (as Table 3) with an explanation of abbreviations. The RSD provides a measure of expected precision, or percentage error, for an analytical method at a given concentration. Comparing the Mean to the MPV MIX can give a qualitative measure of bias for the method at a given concentration.]

*** This is the precision data for your dataset ***
*** at "HOLDING.", hit <CR> to continue listing of data ***

PRECISION DATA BY DATA TYPE AND CONSTITUENT

****

NUM (number of determinations) for each ION and TYP by unique mix
MPV.MIX is theoretical value for the unique mix, with the MEAN,
S.D. (standard deviation), and the RSD (relative standard
deviation, in percent) of the values reported by the laboratory.

****

Values more than 6 std dev from theoretical are deleted

TYP	ION	MPV MIX	NUM	Mean	S.D.	RSD
M	ROE	65.7	8	77.12	8.25	10.70
M	ROE	87.6	14	100.43	15.24	15.17
M	ROE	89.0	3	111.33	3.06	2.74
M	ROE	192.0	5	189.60	6.73	3.55
M	ROE	215.0	5	204.20	7.09	3.47
M	ROE	293.0	3	289.33	19.63	6.78
M	ROE	371.0	7	382.86	27.22	7.11
M	ROE	365.0	9	386.11	31.58	8.18
M	ROE	527.0	8	563.75	26.84	4.76
M	ROE	555.0	7	587.14	43.14	7.35
M	ROE	714.0	8	742.50	67.45	9.08

HOLDING .<CR>

(22) [The program requires several minutes to complete the next step as it generates precision plots. Comments are sent to the screen to indicate that the program is progressing through the step. No interactive input is required.]

```
**************************************************************************
                  Preparing precision plots of the data

There is some inactive terminal time.  Sporadic comments will appear on
the screen to let you know the program is working while plots are being
generated and placed in a file.

Relative Standard Deviation of reported values in percent (REL SD, PCT)
for each unique mix are plotted on the y-axis; and MEAN OF REPORTED
VALUES are plotted on the x-axis
              *** At "HOLDING.." hit <CR> to continue ***
**************************************************************************

     * BEGINNING PLOT STEP NOW *

     * STILL WORKING *

    *** ABOUT HALF WAY THROUGH THIS PLOT STEP ***

     * STILL WORKING - ALMOST DONE *
```

(23) [Precision data from the previous table is plotted. When the program is through generating precision plots it lists the file that is has created. The 'MORE?' prompt after each plot requires interactive input to continue the listing (ie. carriage return). After the listing is complete the user is finished with the QADATA program and returned to the origin directory.]

```
                                       ION = ROE        TYPE = M

                           Plot of RSD by Mean (Legend: *=1, 2=2, ..., $=10+)

           +---+---+---+---+---+---+---+---+---+---+---+---+---+---+---+
       20 +                                                             +
R         |                                                             |
E         |                                                             |
L      15 +        *                                                    +
          |                                                             |
S         |                                                             |
D      10 +      *                                                      +
,         |                               *                           * |
          |                       *       *               *             |
P       5 +                                             *               +
C         |         *     **                                            |
T         |                                                             |
        0 +                                                             +
           +---+---+---+---+---+---+---+---+---+---+---+---+---+---+---+
           0   50 100 150 200 250 300 350 400 450 500 550 600 650 700 750
                                   MEAN OF REPORTED VALUES
```

--More--<u><CR></u>

```
*************************************************************
*        Your session in the BQA data base is finished      *
*************************************************************
```

OK, <u>LO <CR></u>

INTERPRETATION OF PROGRAM OUTPUT

For the next discussion, assume that there are some anomalous dissolved solids data points in a water quality data base analyzed during 1986 that do not fit the historical trend line for a certain area. The user would like to determine if these anomalies can be explained by a problem in laboratory analysis. Statistical output from the two previous examples for retrievals of dissolved solids blind sample data will be used in this section to illustrate how quality-assurance personnel can utilize the QADATA program to evaluate the quality of analytical data produced by the NWQL. In the first example, dissolved solids data for calendar year 1986 is retrieved and a statistical report output to a computer file. In the second example, data is retrieved for a two-month period in 1986 and the results output to the terminal screen.

The quality-assurance data illustrated on the control chart for dissolved solids for calendar year 1986 (fig. 1) suggests that the analytical method was within statistical control most of the year. However, due to a large number of values outside the control limits, results during the September - October period may be questionable. Using the QADATA program a retrieval can be designed for this time period and the statistical output interpreted for precision and accuracy. A retrieval for this two-month period is used in the previous section as an example showing the final report displayed on the terminal screen and step numbers used there are referenced to this example. This study can indicate how much confidence to place in analytical results of environmental samples received from the laboratory during the period.

The control chart for determinations of dissolved solids on blind samples during the September - October period in 1986 (17) indicates a positive bias with several reported values greater than the MPV. Of the 80 values, 30 percent are outside the control limits of two standard deviations and the analytical method is out of statistical control at the 95 percent confidence level for this period (19).

Although the analytical method for dissolved solids has been determined to be out of statistical control, the user should investigate whether the entire concentration range of 66 to 714 mg/L is affected (20). If results from only the very low or very high concentrations are found to be unreliable then results from the the unaffected concentrations can be considered valid. By comparing the mean of the values reported by the laboratory and the MPV of the mix in the table of precision data (21), an indication of bias can be determined for a given concentration. A positive bias is indicated in this data set for low concentrations (less than 100 mg/L) and for high concentrations (370 to 714 mg/L). Based on the lack of bias, results appear to be valid for the mid-range concentrations of 200 to 300 mg/L.

From the QADATA program output, it can be concluded that the analytical method for dissolved solids was out of statistical control during Sepetember - October, 1986, but that analytical results for mid-range concentrations may be valid.

SUMMARY

An interative, menu-driven, user-friendly computer program is available on the Survey's national computer network that allows quality-assurance data users to retrieve results from the blind sample quality assurance program. The QADATA program accesses a data base containing over 50,000 analytical determinations of inorganic and nutrient constituents from the Survey's laboratories in Denver, Colorado, and Ocala, Florida.

Using the QADATA program, the blind sample data for a laboratory can be retrieved from the data base for any user-defined time period for any or all available constituents to meet the needs of specific projects. The program generates a statistical report containing control charts, precision plots, and statistical tables that indicate the quality of analytical data produced by the laboratory. The report can be used to evaluate analytical data produced by the laboratory, to assist in the interpretation of water quality data by explaining anomalous data points, and to document the quality of analytical data produced by the laboratory.

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APPENDIX I - LIST OF CONSTITUENTS AVAILABLE IN QADATA FOR THE NATIONAL WATER-QUALITY LABORATORY

List of constituents (ions) available in blind sample quality-assurance data base for the National Water-Quality Laboratory as provided in the final statistical report output by QADATA.

[dissolved phase; icp = inductively coupled plasma emission spectrometry; aa = atomic absorption spectrometry; col = colorimetry; tot = total recoverable; dcp = direct current plasma.]

MAJORS (milligrams per liter, except Boron in micrograms per liter), TYP = M:

ALK - alkalinity	B - boron	CA - calcium icp
CAAA - calcium aa	CL - chloride	F - fluoride
ROE - dissolved solids (at 180° C)		
MG - magnesium icp	MGAA - magnesium aa	K - potassium
SIO2 - silica icp	SICOL - silica col	NA - sodium icp
NAAA - sodium aa	SO4 - sulfate	

TRACE METALS (micrograms per liter), TYP = T:

AL - aluminum	SB - antimony	AS - arsenic
BA - barium icp	BAAA - barium aa	BAT - barium tot
BE - beryllium icp	BET - beryllium tot	CD - cadmium icp
CDAA - cadmium aa	CDT - cadmium tot	CR - chromium icp
CRDCP - chromium dcp	CRT - chromium tot	CO - cobalt icp
COAA - cobalt aa	COT - cobalt tot	CU - copper icp
CUAA - copper aa	CUT - copper tot	FE - iron icp
FEAA - iron aa	FET - iron tot	PB - lead icp
PBAA - lead aa	PBT - lead tot	LI - lithium icp
LIT - lithium tot	MN - manganese icp	MNAA - manganese aa
MNT - manganese tot	HG - mercury	MO - molybdenum icp
MOAA - molybdenum aa	NI - nickel icp	NIAA - nickel aa
NIT - nickel tot	SE - selenium	AG - silver icp
AGAA - silver aa	AGT - silver tot	SR - strontium
V - vanadium icp	VCOL - vanadium col	ZN - zinc icp
ZNAA - zinc aa	ZNT - zinc tot	

NUTRIENTS (milligrams per liter), TYP = N:

NH4 - ammonia nitrogen as N	KJD - ammonia+organic nitrogen as N
NITR - nitrate+nitrite nitrogen as N	NO2 - nitrite nitrogen as N
PO4 - orthophosphate phosphorus as P	P - phosphorus as P

PRECIPITATION (low-level concentration, milligrams per liter), TYP = P:

NH3 - ammonia nitrogen	CA - calcium	CL - chloride
F - fluoride	MG - magnesium	NO3 - nitrate nitrogen
PO4 - orthophosphate	P - phosphorus	K - potassium
NA - sodium	SPC - specific conductance	SO4 - sulfate

APPENDIX II - LIST OF CONSTITUENTS AVAILABLE IN QADATA FOR THE OCALA WATER QUAILTY SERVICES UNIT

List of constituents (ions) available in blind sample quality-assurance data base for the Ocala WQSU as provided in the final statistical report output by QADATA.

[dissolved phase; aa = atomic absorption spectrometry; col = colorimetry; tot = total recoverable]

MAJORS (milligrams per liter, except Boron in micrograms per liter), TYP = M:

ALK - alkalinity	B - boron	CAAA - calcium aa
CL - chloride	F - fluoride	ROE - dissolved solids (at 180° C)
MGAA - magnesium aa	K - potassium	
SICOL - silica col	NAAA - sodium aa	SO4 - sulfate

TRACE METALS (micrograms per liter), TYP = T:

ALT - aluminum tot	AS - arsenic	BAAA - barium aa
BAT - barium tot	BEAA - beryllium aa	BET - beryllium tot
CDAA - cadmium aa	CDT - cadmium tot	CRDAA - chromium aa
CRT - chromium tot	COAA - cobalt aa	COT - cobalt tot
CUAA - copper aa	CUT - copper tot	FEAA - iron aa
FET - iron tot	PBAA - lead aa	PBT - lead tot
LIT - lithium tot	MNAA - manganese aa	MNT - manganese tot
HG - mercury	MOAA - molybdenum aa	NIAA - nickel aa
NIT - nickel tot	SE - selenium	AGAA - silver aa
AGT - silver tot	SR - strontium	VCOL - vanadium col
ZNAA - zinc aa	ZNT - zinc tot	

NUTRIENTS (milligrams per liter), TYP = N:

NH4 - ammonia nitrogen as N	KJD - ammonia+organic nitrogen as N
NITR - nitrate+nitrite nitrogen as N	NO2 - nitrite nitrogen as N
PO4 - orthophosphate phosphorus as P	P - phosphorus as P

APPENDIX III - LISTING OF COMPUTER CODES FOR USER.CPL

Program USER.CPL is command procedure language that is invoked by entering the command QADATA on QVARSA.

```
&DEBUG &NO_ECHO
term -xoff -FULL
&ARGS USERID
&ARGS USERIDX
&ARGS NODE
&SET_VAR LAB := NWQL
/*Routine checks for a file that is open if program is being used.
&IF [EXISTS BQA>CHECK.COMO -FILE] &THEN &GOTO INUSE
/*Program continues if Check.Como not found
&ELSE &GOTO CONTINUE
&LABEL INUSE
TYPE
TYPE **************************
TYPE RETRIEVAL PROGRAM IS IN USE
TYPE PLEASE TRY AGAIN LATER
TYPE **************************
TYPE
OR
&RETURN
&LABEL CONTINUE
COMO BQA>CHECK.COMO
OPEN T$0000 101 2
CLOSE T$0000
DELETE T$0000
TYPE .
TYPE WELCOME TO THE BLIND SAMPLE INTERACTIVE RETRIEVAL PROGRAM
TYPE .
TYPE ************************************************************************
TYPE .
TYPE USERID:        needed to tag data files.
TYPE .
TYPE PRIME NODE:    needed as a destination for output data file.
TYPE .
TYPE ************************************************************************
TYPE .
&LABEL AGAIN
&IF [NULL %USERIDX%]~
  &THEN &SET_VAR USERIDX := [RESPONSE 'Enter your userid']
TYPE .
&IF [NULL %NODE%]~
  &THEN &SET_VAR NODE := [RESPONSE 'Enter your PRIME node']
/*If response to userid is null, user is prompted again.
&IF [NULL %USERIDX%] &THEN &GOTO AGAIN
/*Userid is limited to ten characters so filenames do not exceed
/*32 character limit for fts.
&SET_VAR USERID := [SUBSTR %USERIDX% 1 10]
COMO -E
COMO BQA>USER.COMO.%USERID%
```

```
A BQA>INFO.DIR
/*INFO is invoked with userid QAD to run QAMENU-PGM
&DATA INFO
  QAD
  RUN QAMENU-PGM
&TTY
&END
/*If error in cpl program goes to routine error_path and terminates.
&SEVERITY &ERROR &ROUTINE ERROR_PATH
/*User chooses output type for final report - screen or computer file.
TYPE ************************************************************************
TYPE YOUR DATASET IS READY TO ENTER THE PLOT PORTION OF THE PROGRAM
TYPE ************************************************************************
TYPE At the next prompt, please answer "YES" or "NO":
TYPE .
TYPE YES = plots and tables are output to the terminal screen in 80-column
TYPE format. PLEASE DO NOT USE THIS OPTION IF YOUR RETRIEVAL CONTAINS MORE
THAN
TYPE TWO CONSTITUENTS!  This option is only recommended for small retrievals
TYPE since large datasets can affect response time for other users on the
TYPE system.  Your terminal will remain in interactive mode and will require
TYPE keyboard input for several prompts during the session.  Plots and tables
TYPE are NOT output to a file on the PRIME.
TYPE .
TYPE NO = plots and tables are NOT output to the screen but are output to a
TYPE plot file in 132-column format and transferred to the fts_depot at your
TYPE PRIME. A system phantom finishes the program without interactive input.
TYPE ************************************************************************
TYPE .
/*If 'yes' to this query, cpl continues output to the terminal screen
/*in interactive mode.  Statistical report to the screen.
&IF [QUERY 'DO YOU WANT TO VIEW PLOTS ON YOUR TERMINAL SCREEN']~
  &THEN &GOTO SCREEN_PLOTS
/*WHEN USER ANSWERS PROMPT, REPORT IS TAGGED WITH PROPER LAB NAME
TYPE .
TYPE PLEASE ANSWER 'YES' OR 'NO' TO THE NEXT PROMPT:
TYPE .
&IF [QUERY 'DID YOU RETRIEVE DATA FOR THE OCALA WQSU LABORATORY']™
  &THEN &SET_VAR LAB : = OCALA

/*Variables containing userid, node, and labname are read to a file so
/*the phantom will be able to use them in generating filenames.
&DATA ED

I %USERID%
FILE USERID

&END
&DATA ED

I %NODE%
FILE NODE

&END
```

```
&DATA ED

I %LAB%
FILE LABNAME

&END
/*Phantom generates final report and sends it to user's computer node
PH BQA>USERPH.CPL
TYPE ************************************************************************
TYPE * A system phantom will now generate a final file of your dataset     *
TYPE * and transfer it to your fts_depot as QAPLOTS.your userid.date.time  *
TYPE * Copies of your DATA and PLOT files will be saved in USER.DIR in     *
TYPE * case they are lost in the process.  If you need assistance contact  *
TYPE * Keith Lucey KJLUCEY at FTS 776-1491 or comm 303-236-1491.           *
TYPE ************************************************************************
/*After phantom is invoked, this cpl terminates in last_step routine
&GOTO LAST_STEP
/*CPL continues at this step for screen output of statistical report
&LABEL SCREEN_PLOTS
TYPE ************************************************************
TYPE *  The following step prepares the data for the plot step  *
TYPE *            It can take a while - be patient              *
TYPE ************************************************************
/*INFO output is edited to be compatible with PSTAT
CN QADNSP SD.DATA
&DATA ED SD.DATA
BRIEF
TOP
L \;C/\/ /G;*
FILE SD.DATA
Q
&END
/*File of retrieved QA data is saved
COPY SD.DATA BQA>USER.DIR>%USERID%.QADAT.[DATE -FTAG]
/*Invoke pstat and load transfer file
&DATA PSTAT
 TRANSFER QA.TRANS$
&TTY
&END
TYPE ************************************************************
TYPE ** Plot file is being edited - hit <CR> at the MORE? prompt **
TYPE ************************************************************
/*Plot file of precision plots generated by PSTAT have to be edited
/*so PLIST can scroll them on the terminal screen
&DATA ED PLOTS.CV.SCR
BRIEF
LOC There;DELETE;*
TOP
LOC MEAN;LOC 1;I ^214;*
BOT
I X
I X
FILE
&TTY
```

```
&END
/*Precision plots are scrolled
PLIST PLOTS.CV.SCR
DELETE (PLOTS.CV.SCR SD.DATA)
/*File check.como is deleted at termination of the session and the
/*QADATA program is now available to other users
DELETE BQA>CHECK.COMO
&LABEL LAST_STEP
TYPE ********************************************************************
TYPE *            Your session in the BQA data base is finished          *
TYPE ********************************************************************
OR
COMO -E
&RETURN
/*If the cpl finds an error, such as a null retrieval, the program
/*terminates normally and the user can re-enter and try again.
&ROUTINE ERROR_PATH
COMO BQA>ERROR.COMO
DATE
TYPE .
TYPE There was a problem with the retrieved dataset and no output will
TYPE be generated.  You can try another retrieval.  Enter QADATA.
TYPE .
DELETE (BQA>CHECK.COMO BQA>INFO.DIR>SD.DATA)
&GOTO LAST_STEP
COMO -E
&RETURN
```

APPENDIX IV - LISTING OF COMPUTER CODES FOR QAMENU.PGM

Program QAMENU.PGM contains INFO programming language that allows interactive input to define the retrievals from the blind sample data base.

```
/*Initial formatting of variables.
FORMAT $NUM11,8,N,0
FORMAT $NUM12,8,N,0
FORMAT $CHR21,6,C
FORMAT $CHR25,2,C
DFMT MDY\-
CALCULATE $PRINTER-SIZE=132
CALCULATE $CASE-FLAG=2
CALCULATE $NUM4=0
CALCULATE $NUM7=0
/*Introductory screen explaining program
DIS =
DIS '                      BRANCH OF QUALITY ASSURANCE'
DIS ''
DIS '                   DATA BASE FOR BLIND SAMPLE PROJECT'
DIS ''
DIS
'*************************************************************************'
DIS ''
DIS '  This program allows you to access the blind sample quality-assurance'
DIS '  data base for the National Water Quality Laboratory and the data base'
DIS '  for the laboratory of the Water Quality Services Unit in Ocala'
DIS '  for any or all of several inorganic constituents (major ions, trace'
DIS '  metals, nutrients, and low-level concentration precipitation samples)'
DIS '  for any time period that you define in the last five water-years. '
DIS ''
DIS '  Control charts, precision plots, and several statistical tables will'
DIS '  be generated, which will indicate the quality of the analytical data'
DIS '  produced by the laboratory during the time period that you request.'
DIS ''
DIS '  The program will prompt for the necessary information.  Please be'
DIS '  sure your keyboard is in the "CAPS LOCK" mode.'
DIS ''
DIS '           (hit "return" or enter any key to continue)'
CURSOR 21,60
/*Program needs keyboard input in response to prompt
ACCEPT $CHR24
LABEL LABS
/*Screen to access data base
DIS =
CURSOR 5,5
DIS ''
DIS '            FOR HELP CONTACT KEITH J. LUCEY (KJLUCEY)'
DIS '                FTS 776-1491 OR COMM 303-236-1491'
DIS '*************************************************************'
DIS ''
DIS ''
DIS '    BE SURE YOUR KEYBOARD IS IN THE "CAPS LOCK" MODE'
```

```
DIS '    (Retrieve data for only one laboratory per login session).'
DIS ''
DIS '    Then choose one of the following:'
DIS ''
DIS '    Enter any key or "return" = access NWQL QA data base'
DIS '    Enter 33                  = access Ocala WQSU QA data base'
DIS '    Enter 99                  = no more retrievals, exit program'
CURSOR 14,50
ACCEPT $CHR22
/*If response is '99' flow to routine FINI to exit program
IF $CHR22 EQ '99'
 GOTO FINI
ENDIF
/*Program selects ACSII file containing data base which is sorted
/*by date, type, date, ion.
SELECT MASTER.DAT
LABEL AGAIN
DIS =
CURSOR 10,10
DIS 'QUALITY-ASSURANCE DATABASE FOR ROUTINE WATER-ANALYSES'
DIS ''
DIS '           What type of QA data would you like to access?'
DIS '         (there is no precipitation data for the Ocala WQSU)'
DIS ''
DIS '                      M  =  MAJOR IONS    '
DIS '                      T  =  TRACE METALS  '
DIS '                      N  =  NUTRIENTS     '
DIS '                      P  =  PRECIPITATION (LIS)'
DIS ''
DIS '           Select one type or "99" to exit program'
CURSOR 19,60
ACCEPT $CHR25
/*User chooses one data type and data base is reselected
IF $CHR25 EQ '99'
   GOTO FINI
ENDIF
IF $CHR25 EQ 'M'
   RESELECT BY TYPE = 'M'
   GOTO DATES
ENDIF
IF $CHR25 EQ 'T'
   RESELECT BY TYPE = 'T'
   GOTO DATES
ENDIF
IF $CHR25 EQ 'N'
   RESELECT BY TYPE = 'N'
   GOTO DATES
ENDIF
IF $CHR25 EQ 'P'
   RESELECT BY TYPE = 'P'
   GOTO DATES
ENDIF
GOTO AGAIN
LABEL DATES
```

```
DIS =
CURSOR 5,10
DIS '   AVAILABILITY OF QUALITY-ASSURANCE DATA TYPES '
DIS ''
                                NWQL                    WQSU
DIS ''
DIS '        MAJORS          1985 - present          1989 - present'
DIS '        TRACE METALS    1985 - present          1989 - present'
DIS '        NUTRIENTS       1986 - present          1989 - present'
DIS '        PRECIPS         1986 -'
DIS ''
DIS '     (most current data is 1 - 2 months prior to the present)'
DIS ''
DIS 'Enter the beginning and ending login dates for your period of interest'
DIS 'using the yyyymmdd format (ie. 19881019 = October 19, 1988).'
DIS ''
DIS 'Beginning date:'
/*User enters date in proper format.
CURSOR 17,18
ACCEPT $NUM11
CURSOR 19,1
DIS 'Ending date:'
CURSOR 19,15
ACCEPT $NUM12
/*If beginning date not less than ending date for retrieval, user
/*is returned to DATES routine for another try.
IF $NUM12 LT $NUM11
  DIS =
  CURSOR 5,10
  DIS 'PLEASE HAVE YOUR BEGINNING DATE LESS THAN THE ENDING DATE'
  SLEEP 2
  GOTO DATES
ENDIF
IF $NUM12 = $NUM11
  DIS =
  CURSOR 5,10
  DIS 'PLEASE REENTER BEGINNING DATE AND ENDING DATE'
  SLEEP 2
  GOTO DATES
ENDIF
LABEL REDO
/*Master.dat is reselected for retrieval dates
RESELECT BY LIDATE GE $NUM11
RESELECT BY LIDATE LE $NUM12
DIS =
CURSOR 5,10
DIS $NOSEL, ' RECORDS SELECTED'
SLEEP 2
DIS =
IF $CHR25 EQ 'M'
  GOTO MAJ
ENDIF
IF $CHR25 EQ 'T'
  GOTO TRC
```

```
ENDIF
IF $CHR25 EQ 'N'
  GOTO NUTR
ENDIF
IF $CHR25 EQ 'P'
  GOTO PPT
ENDIF
/*Routine to choose major ion constituents
LABEL MAJ
CURSOR 2,5
DIS 'CHOOSE THE "ALL" OPTION TO RETRIEVE DATA FOR ALL MAJOR CONSTITUENTS.'
DIS '    YOU CAN CHOOSE CONSTITUENTS INDIVIDUALLY USING THE INDICATED PROMPT.'
DIS '              (all constituents in dissolved phase)'
DIS ''
DIS '         (icp = inductively coupled emission spectrometry)'
DIS '              (aa = atomic absorption spectrometry)'
DIS ''
DIS '    ALK - alkalinity              B - boron'
DIS '    CA - calcium icp              CAAA - calcium aa'
DIS '    CL - chloride                 ROE - dissolved solids (at 180# C)'
DIS '    F - fluoride                  MG - magnesium icp'
DIS '    MGAA - magnesium aa           K - potassium'
DIS '    SIO2 - silica icp             SICOL - silica, colorimetry'
DIS '    NA - sodium icp               NAAA - sodium aa'
DIS '    SO4 - sulfate                 ALL - retrieve all major constituents'
DIS ''
DIS '            Choose only one: (return to end)'
CURSOR 18,51
GOTO IONS
/*Routine to retrieve trace metal constituents
LABEL TRC
CURSOR 1,3
DIS 'CHOOSE THE "ALL" OPTION TO RETRIEVE FOR EVERY TRACE METAL CONSTITUENT'
DIS '   OR YOU CAN RETRIEVE INDIVIDUALLY BY USING THE INDICATED PROMPT.'
DIS '************(dissolved data unless otherwise noted).******************'
DIS '    (icp = inductively coupled plasma emission spectrometry)'
DIS '    (aa = atomic absorption spectrometry;  tot = total recoverable)'
DIS '    (dcp = direct current plasma;          col = colorimetry)'
DIS ' AL - aluminum          SB - antimony          AS - arsenic'
DIS ' BA - barium icp        BAAA - barium aa       BAT - barium tot'
DIS ' BE - beryllium icp     BET - beryllium tot    CD - cadmium icp'
DIS ' CDAA - cadmium aa      CDT - cadmium tot      CR - chromium icp'
DIS ' CRDCP - chromium dcp   CRT - chromium tot     CO - cobalt icp'
DIS ' COAA - cobalt aa       COT - cobalt tot       CU - copper icp'
DIS ' CUAA - copper aa       CUT - copper tot       FE - iron icp'
DIS ' FEAA - iron aa         FET - iron tot         PB - lead icp'
DIS ' PBAA - lead aa         PBT - lead tot         LI - lithium icp'
DIS ' LIT - lithium tot      MN - manganese icp     MNAA - manganese aa'
DIS ' MNT - manganese tot    HG - mercury           MO - molybdenum icp'
DIS ' MOAA - molybdenum aa   NI - nickel icp        NIAA - nickel aa'
DIS ' NIT - nickel tot       SE - selenium          AG - silver icp'
DIS ' AGAA - silver aa       AGT - silver tot       V - vanadium icp'
DIS ' VCOL - vanadium col    SR - strontium         ZN - zinc icp'
DIS ' ZNAA - zinc aa         ZNT - zinc tot         ALL - all constituents'
```

```
DIS '            Choose only one: (return to end)'
CURSOR 23,53
GOTO IONS
/*Routine to retrieve nutrient constituents
LABEL NUTR
CURSOR 5,5
DIS 'IF YOU WANT DATA FOR ALL OF THE FOLLOWING NUTRIENT CONSTITUENTS,'
DIS '     CHOOSE THE "ALL" OPTION; YOU CAN CHOOSE CONSTITUENTS ON'
DIS '     AN INDIVIDUAL BASIS USING THE INDICATED PROMPT.'
DIS ''
DIS ' (includes dissolved and total values - no difference in methods)'
DIS ''
DIS '       NH4 - ammonia nitrogen as N'
DIS '       KJD - ammonia + organic nitrogen as N'
DIS '      NITR - nitrate + nitrite nitrogen as N'
DIS '       NO2 - nitrite nitrogen as N'
DIS '       PO4 - orthophosphate phosphorus as P'
DIS '         P - phosphorus as P'
DIS '       ALL - retrieve all nutrient constituents'
DIS ''
DIS '            Choose only one: (return to end)'
CURSOR 19,53
GOTO IONS
/*Routine to retrieve precip constituents (low-ionic strength)
LABEL PPT
CURSOR 5,5
DIS 'CHOOSE THE "ALL" OPTION TO RETRIEVE DATA FOR ALL PRECIPITATION'
DIS '    (low-level concentration) CONSTITUENTS.  YOU CAN CHOOSE '
DIS '    CONSTITUENTS INDIVIDUALLY BY USING THE INDICATED PROMPT.'
DIS ''
DIS '  NH3 - ammonia nitrogen          CA  - calcium'
DIS '  CL  - chloride                  F   - fluoride'
DIS '  MG  - magnesium                 NO3 - nitrate nitrogen'
DIS '  PO4 - orthophosphate            P   - phosphorus'
DIS '  K   - potassium                 NA  - sodium'
DIS '  SPC - specific conductance      SO4 - sulfate'
DIS '  ALL - retrieve all constituents'
DIS ''
DIS '            Choose only one: (return to end)'
CURSOR 17,53
/*Routine accepts input from constituent retrieval screens.
/*If response is null, ALL, or END goes to routine CONTIN
LABEL IONS
ACCEPT $CHR21
IF $CHR21 EQ '0'
  GOTO CONTIN
ENDIF
IF $CHR21 EQ 'ALL'
  GOTO CONTIN
ENDIF
IF $CHR21 EQ 'END'
  GOTO CONTIN
ENDIF
DIS =
```

```
CURSOR 10,10
DIS 'This step sometimes takes several seconds'
/*Data base is reselected for ion chosen.
RESELECT FOR ION = $CHR21
LABEL CONTIN
DIS =
CURSOR 2,5
DIS 'THIS PORTION OF YOUR RETRIEVAL IS',$NOSEL,' RECORDS:'
DIS ''
DIS ''
DIS 'This step may take a few seconds - wait for the next prompt'
SLEEP 3
/*Retrieved data is placed in the QADNSP file
PRINT ION,TYPE,LIDATE,MIX,VAL,MPV,SD,NSD
/*If user chose ALL constituents program goes to exit screen
IF $CHR21 = 'ALL'
  GOTO EXIT
ENDIF
/*If individual constituents are chosen, user can choose to
/*return to the constituent list and retrieve data for other
/*constituents in the next routine
DIS =
CURSOR 5,5
IF $CHR25 EQ 'M'
  DIS 'Do you want to retrieve more majors for this period?'
  DIS '     1 = yes, 2 = no'
ENDIF
IF $CHR25 EQ 'T'
  DIS 'Do you want to retrieve more traces for this period?'
  DIS '     1 = yes, 2 = no'
ENDIF
IF $CHR25 EQ 'N'
  DIS 'Do you want to retrieve more nutrients for this period?'
  DIS '     1 = yes, 2 = no'
ENDIF
IF $CHR25 EQ 'P'
  DIS 'Do you want to retrieve more precips for this period?'
  DIS '     1 = yes, 2 = no'
ENDIF
CURSOR 6,35
ACCEPT $NUM4
/*A YES response causes INFO to reselect the retrieved data by type
/*and the user is sent to routine REDO to continue the session
IF $NUM4 EQ 1
 NSELECT
 RESELECT BY TYPE = $CHR25
 GOTO REDO
ENDIF
IF $NUM4 EQ 99
  END
ENDIF
/*This screen explains that the user will be returned to the screen
/*where a new retrieval can be defined or the program terminated
LABEL EXIT
```

```
DIS =
CURSOR 5,5
DIS 'You have finished your retrieval of this range of QA data.'
DIS '    You will now be returned to the initial program setup where'
DIS '    you can either continue retrieving data from the other types'
DIS '    of QA data or leave the retrieval portion of the program.'
DIS ''
DIS '    ONLY RETRIEVE DATA FOR ONE LABORATORY PER TERMINAL SESSION.'
DIS ''
DIS '          (hit "return" or enter any key to continue)'
ACCEPT $CHR23
GOTO LABS
/*This screen explains status of data files.
LABEL FINI
DIS =
CURSOR 5,6
DIS 'A file of the data that you have retrieved will be saved in our '
DIS '     USER.DIR as "(your userid).QADATA.(date).(time)" for one week.'
DIS '     This file contains the raw QA data and you can get a copy from'
DIS '     Blind Sample Project personnel.'
DIS ''
DIS '     The program will now prepare control and precision charts'
DIS '     for your data. You can choose to have the final data report'
DIS '     displayed at your terminal screen or transferred to your'
DIS '     PRIME as "FTS_DEPOT>QAPLOTS.(your userid).(date).(time)".'
DIS ''
DIS '     PLEASE NOTE:  OUTPUT TO THE SCREEN SHOULD ONLY BE USED'
DIS '                   FOR RETRIEVALS OF ONE OR TWO CONSTITUENTS'
DIS ''
DIS '           (hit "return" or enter any key to continue)'
ACCEPT $CHR20
Q STOP
/*INFO session terminates and control is returned to USER.CPL
```

APPENDIX V - LISTING OF COMPUTER CODES FOR QA1.TRANS

Program QA1.TRANS: P-STAT commands that generate statistical tables and plots of retrieved data set and outputs them to the terminal screen.

```
MAXERROR 888 $
VERBOSITY 1 $
TEXT;
*** Your dataset is being loaded into the plot program ***
$
/*Pstat file is created from ASCII file SD.DATA
BUILD SD.P, END.OF.CASE OFF,
VARS ION:C TYP:C MONTH DAY YEAR MIX:C VAL MPV SD NSD,
FILE SD.DATA,
MISSING ' . '
$
TEXT;
*** computing decimal date for control charts ***
     *** (ie. 3.5 = Mar 15; 4 = Apr 1;) ***
$
/*Date values are computed from julian and precip constituents are
/*re-labelled to be distinguished from those in major ions
MODIFY SD.P
(GEN DECIMAL.DATE = MONTH + DAY/30)
(IF TYP = 'P' AND ION = 'CA', SET ION = 'CA.P')
(IF TYP = 'P' AND ION = 'CL', SET ION = 'CL.P')
(IF TYP = 'P' AND ION = 'F', SET ION = 'F.P')
(IF TYP = 'P' AND ION = 'K', SET ION = 'K.P')
(IF TYP = 'P' AND ION = 'MG', SET ION = 'MG.P')
(IF TYP = 'P' AND ION = 'NA', SET ION = 'NA.P')
(IF TYP = 'P' AND ION = 'P', SET ION = 'PHOS.P')
(IF TYP = 'P' AND ION = 'PO4', SET ION = 'PO4.P')
(IF TYP = 'P' AND ION = 'SO4', SET ION = 'SO4.P'),
OUT SD.P,
REPLACE$
/*Data is sorted for plot step
SORT SD.P,
BY TYP ION YEAR,
OUT SD.P,
REPLACE$
TEXT;
*** CONTROL CHARTS WILL FOLLOW - PLEASE NOTE THESE ABBREVIATIONS      ***
    TYP = data type (M - majors, N - nutrients, P - precipitation
    samples, T - trace metals);  NSD = number of standard deviations;
    MPV = most probable value or theoretical value.  Date on x-axis
    is decimal.date, ie. 1 = Jan 1, 6.5 = June 15, 11.7 = November 21

*** At "HOLDING.." hit <CR> to continue ***
$
/*Control charts with NSD values set to max 6 and min -6
PLOT SD.P (IF NSD > 6, SET NSD = 6)
(IF NSD < -6, SET NSD = -6),
BY TYP ION YEAR;
PLOT NSD * DECIMAL.DATE, TICKS Y -6 TO 6 BY 2,
```

```
GRID.LINES Y -2 TO 2 BY 2, LABEL X 'DATE SAMPLE LOGGED INTO LABORATORY',
LABEL Y 'NSD FROM MPV';
$
TEXT;
            *** computing data for precision plots ***
$
/*Data resorted
SORT SD.P,
BY TYP ION MIX,
OUT CV.SORT
$
PURGE SD.P$
TEXT;
*************************************************************************
   Preparing display of constituents with total number of obs (TOT.NUM),
   number > 2 s.d. (NUM.2SD), and number > 6 s.d. (NUM.6SD).

   Values greater than 6 standard deviations from the theoretical
   will be deleted from the dataset before calculating relative
   standard deviation and plotting of precision data.

            *** At "HOLDING.." hit <CR> to continue ***
*************************************************************************
$
/*This step counts number of values greater than 2 and 6 s.d.
AGGREGATE CV.SORT (KEEP TYP ION NSD)
(IF NSD>2 OR NSD<-2, GEN SD2=1)
(IF NSD>6 OR NSD<-6, GEN SD6=1),
COLLECT,
COUNT,
BY TYP ION,
OUT QA.COUNTS $
/*Percentages of total are calculated for values generated in the
/*AGGREGATE step
MODIFY QA.COUNTS (RENAME n.SD2 = NUM.SD2)
(RENAME n.SD6 = NUM.SD6) (RENAME n.NSD = TOT.NUM)
(GEN PERCENT.OVER.2SD = NUM.SD2/TOT.NUM*100)
(GEN PERCENT.OVER.6SD = NUM.SD6/TOT.NUM*100),
OUT QA.COUNTS,
REPLACE$
/*Title of table to be displayed on the terminal screen
TITLE T1 'CONSTITUENTS IN RETRIEVAL WITH NUMBER OF DETERMINATIONS'$
TITLE T2 '*************************************************************'$
TITLE T3 'TYP = data type, M=major, T=trace metal, N=nutrient, P=precip'$
TITLE T4 'TOT.NUM = total number of determinations'$
TITLE T5 'NUM.2SD = number > 2 standard deviations from theoretical  '$
TITLE T6 'NUM.6SD = number > 6 standard deviations from theoretical  '$
/*Table is listed to terminal screen
LIST QA.COUNTS, TITLE, PLACES 1
$
PURGE QA.COUNTS$
TITLES RESET$
TEXT;
*** More computing ***
```

```
$
/*Outliers are excluded from dataset for precision data
MODIFY CV.SORT (IF NSD > 6, EXCLUDE) (IF NSD < -6, EXCLUDE),
OUT CV.SORT,
REPLACE$
/*Precision data calculated
PERCENTILES CV.SORT (KEEP TYP ION MIX MPV VAL),
DES CV.DES,
BY TYP ION MIX MPV
$
/*Range of mpv's determined
PERCENTILES CV.SORT (KEEP TYP ION MPV),
DES MPV.DES,
BY TYP ION
$
TEXT;
             *** At "HOLDING.." hit <CR> to continue ***
$
/*Pertinent data is kept from mpv description file
MODIFY MPV.DES (KEEP TYP ION LOW HIGH),
OUT MPV.DES,
REPLACE$
TEXT;
*** Range of theoretical values (MPV's) in your dataset ***
         *** At "HOLDING.." hit <CR> to continue ***
$
/*New title for mpv table
TITLE T1 'RANGE OF THEORETICAL CONCENTRATIONS (MPV) BY CONSTITUENT'$
TITLE T2 '*************************************************************'$
TITLE T3 'TYP = data type: M=majors, T=trace metals, N=nutrients, P=precips'$
TITLE T4 'HIGH and LOW values reported in milligrams per liter, except for '$
TITLE T5 'trace metals (T) and boron (B) which are in micrograms per liter.'$
/*Table of MPV ranges is displayed on screen
LIST MPV.DES, TITLE
$
PURGE MPV.DES$
PURGE CV.SORT$
/*RSD values are generated from cv.des file and variables renamed
MODIFY CV.DES (KEEP TYP ION MPV GOOD MEAN S.D.)
(GEN RSD=S.D./MEAN*100) (RENAME GOOD TO NUM) (RENAME MPV TO MPV.MIX),
OUT CV.DES,
REPLACE$
SORT CV.DES,
BY TYP ION MEAN,
OUT CV.DES,
REPLACE$
TEXT;
    *** This is the precision data for your dataset ***
*** at "HOLDING.", hit <CR> to continue listing of data ***
$
/*New title for precision table
TITLE T1 'PRECISION DATA BY DATA TYPE AND CONSTITUENT'$
TITLE T2 '*************************************************************'$
TITLE T3 'NUM (number of determinations) for each ION and TYP by unique mix'$
```

```
TITLE T4 'MPV.MIX is theoretical value for the unique mix, with the MEAN,   '$
TITLE T5 'S.D. (standard deviation), and the RSD (relative standard         '$
TITLE T6 'deviation, in percent) of the values reported by the laboratory.  '$
TITLE T7 '*************************************************************'$
TITLE T8 'Values more than six std dev from theoretical are deleted'$
/*Precision data listed to screen if more than two determinations
LIST CV.DES (IF NUM > 2, CONTINUE), TITLE, PLACES 2
$
TITLES RESET $
TEXT;
*****************************************************************************
               Preparing precision plots of the data

     There is some incactive terminal time.  Sporadic comments will
     appear on the screen to let you know the program is working
     while plots are being generated and placed in a file.

 Relative Standard Deviation of reported values in percent
 (REL SD, PCT) for each unique mix are plotted on the y-axis;
 and MEAN OF REPORTED VALUES are plotted on the x-axis

            *** At "HOLDING.." hit <CR> to continue ***
*****************************************************************************
$
BATCH $
VERBOSITY 1 $
LINES 22 $
/*Plot file is set up with proper width for screen
PRINT.PARAMETERS PLOTS.CV.SCR, OUTPUT.WIDTH 78, NO ECHO $
ERROR SHORT $
/*This macro is called for each constituent to generate precision plots.
/*Plot step sets RSD to max of 100 and data is excluded if number
/*of determinations is less than three
MACRO PLOTS $
PLOT CV.DES (IF RSD>100, SET RSD=100)
(IF ION = 'XXXXXX', CONTINUE) (IF NUM < 3, EXCLUDE);
PLOT RSD*MEAN, EDGES T B L R, TITLES T2 CENTER
 '      ION = XXXXXX        TYPE = ZZ', LABEL X 'MEAN CONCENTRATION',
LABEL X 'MEAN OF REPORTED VALUES', LABEL Y 'REL SD, PCT',
PRINTER PLOTS.CV.SCR;
$
MACEND$
TEXT;
 * BEGINNING PLOT STEP NOW *
$
/*Repeatedly call macro PLOTS
RUN PLOTS, XXXXXX ALK, ZZ M $
RUN PLOTS, XXXXXX B, ZZ M $
RUN PLOTS, XXXXXX CA, ZZ M $
RUN PLOTS, XXXXXX CAAA, ZZ M $
RUN PLOTS, XXXXXX CL, ZZ M $
RUN PLOTS, XXXXXX ROE, ZZ M $
RUN PLOTS, XXXXXX F, ZZ M $
RUN PLOTS, XXXXXX MG, ZZ M $
```

```
RUN PLOTS, XXXXXX MGAA, ZZ M $
RUN PLOTS, XXXXXX K, ZZ M $
RUN PLOTS, XXXXXX SIO2, ZZ M $
RUN PLOTS, XXXXXX SICOL, ZZ M $
RUN PLOTS, XXXXXX NA, ZZ M $
RUN PLOTS, XXXXXX NAAA, ZZ M $
RUN PLOTS, XXXXXX SO4, ZZ M $
TEXT;
 * STILL WORKING *
$
RUN PLOTS, XXXXXX NH4, ZZ N $
RUN PLOTS, XXXXXX KJD, ZZ N $
RUN PLOTS, XXXXXX NITR, ZZ N $
RUN PLOTS, XXXXXX NO2, ZZ N $
RUN PLOTS, XXXXXX P, ZZ N $
RUN PLOTS, XXXXXX PO4, ZZ N $
RUN PLOTS, XXXXXX CA.P, ZZ P $
RUN PLOTS, XXXXXX CL.P, ZZ P $
RUN PLOTS, XXXXXX F.P, ZZ P $
RUN PLOTS, XXXXXX K.P, ZZ P $
RUN PLOTS, XXXXXX MG.P, ZZ P $
RUN PLOTS, XXXXXX NH3, ZZ P $
RUN PLOTS, XXXXXX NO3, ZZ P $
RUN PLOTS, XXXXXX PO4.P, ZZ P $
RUN PLOTS, XXXXXX PHOS.P, ZZ P $
RUN PLOTS, XXXXXX NA.P, ZZ P $
RUN PLOTS, XXXXXX SO4.P, ZZ P $
RUN PLOTS, XXXXXX SPC, ZZ P $
TEXT;
*** ABOUT HALF WAY THROUGH THIS PLOT STEP ***
$
RUN PLOTS, XXXXXX AL, ZZ T $
RUN PLOTS, XXXXXX SB, ZZ T $
RUN PLOTS, XXXXXX AS, ZZ T $
RUN PLOTS, XXXXXX BA, ZZ T $
RUN PLOTS, XXXXXX BAAA, ZZ T $
RUN PLOTS, XXXXXX BAT, ZZ T $
RUN PLOTS, XXXXXX BE, ZZ T $
RUN PLOTS, XXXXXX BET, ZZ T $
RUN PLOTS, XXXXXX CD, ZZ T $
RUN PLOTS, XXXXXX CDAA, ZZ T $
RUN PLOTS, XXXXXX CDT, ZZ T $
RUN PLOTS, XXXXXX CR, ZZ T $
RUN PLOTS, XXXXXX CRDCP, ZZ T $
RUN PLOTS, XXXXXX CRT, ZZ T $
RUN PLOTS, XXXXXX CO, ZZ T $
RUN PLOTS, XXXXXX COAA, ZZ T $
RUN PLOTS, XXXXXX COT, ZZ T $
RUN PLOTS, XXXXXX CU, ZZ T $
RUN PLOTS, XXXXXX CUAA, ZZ T $
RUN PLOTS, XXXXXX CUT, ZZ T $
RUN PLOTS, XXXXXX FE, ZZ T $
RUN PLOTS, XXXXXX FEAA, ZZ T $
RUN PLOTS, XXXXXX FET, ZZ T $
```

```
RUN PLOTS, XXXXXX PB, ZZ T $
RUN PLOTS, XXXXXX PBAA, ZZ T $
RUN PLOTS, XXXXXX PBT, ZZ T $
TEXT;
 * STILL WORKING - ALMOST DONE *
$
RUN PLOTS, XXXXXX LI, ZZ T $
RUN PLOTS, XXXXXX LIT, ZZ T $
RUN PLOTS, XXXXXX MN, ZZ T $
RUN PLOTS, XXXXXX MNAA, ZZ T $
RUN PLOTS, XXXXXX MNT, ZZ T $
RUN PLOTS, XXXXXX HG, ZZ T $
RUN PLOTS, XXXXXX MO, ZZ T $
RUN PLOTS, XXXXXX MOAA, ZZ T $
RUN PLOTS, XXXXXX NI, ZZ T $
RUN PLOTS, XXXXXX NIAA, ZZ T $
RUN PLOTS, XXXXXX NIT, ZZ T $
RUN PLOTS, XXXXXX SE, ZZ T $
RUN PLOTS, XXXXXX AG, ZZ T $
RUN PLOTS, XXXXXX AGAA, ZZ T $
RUN PLOTS, XXXXXX AGT, ZZ T $
RUN PLOTS, XXXXXX SR, ZZ T $
RUN PLOTS, XXXXXX V, ZZ T $
RUN PLOTS, XXXXXX VCOL, ZZ T $
RUN PLOTS, XXXXXX ZN, ZZ T $
RUN PLOTS, XXXXXX ZNAA, ZZ T $
RUN PLOTS, XXXXXX ZNT, ZZ T $
PURGE CV.DES$
END$
/*Control is returned to USER.CPL where PLOTS.CV.SCR is listed on the
/*terminal screen
```

APPENDIX VI - LISTING OF COMPUTER CODES FOR QA.TRANS

Program QA.TRANS: P-STAT commands that generate statistical tables and plots of retrieved data set that are output to ASCII files where the USERPH.CPL compiles a final report to be transferred to the office designated by the user.

```
MAXERROR 888 $
VERBOSITY 1 $
ERROR SHORT $
TEXT;
*** YOUR DATASET IS BEING LOADED INTO THE PLOT PROGRAM ***
$
/*File is created from ASCII file SD.DATA
BUILD SD.P, END.OF.CASE OFF,
VARS ION:C TYP:C MONTH DAY YEAR MIX:C VAL MPV SD NSD,
FILE SD.DATA,
MISSING ' . '
$
TEXT;
*** DATA IS BEING PREPARED FOR CONTROL CHARTS - PLEASE BE PATIENT ***
$
/*Date values are generated from julian dates and precip ions
/*are renamed to distinguish from major ions
MODIFY SD.P
(GEN DECIMAL.DATE = MONTH + DAY/30)
(IF TYP = 'P' AND ION = 'CA', SET ION = 'CA.P')
(IF TYP = 'P' AND ION = 'CL', SET ION = 'CL.P')
(IF TYP = 'P' AND ION = 'F', SET ION = 'F.P')
(IF TYP = 'P' AND ION = 'K', SET ION = 'K.P')
(IF TYP = 'P' AND ION = 'MG', SET ION = 'MG.P')
(IF TYP = 'P' AND ION = 'NA', SET ION = 'NA.P')
(IF TYP = 'P' AND ION = 'P', SET ION = 'PHOS.P')
(IF TYP = 'P' AND ION = 'PO4', SET ION = 'PO4.P')
(IF TYP = 'P' AND ION = 'SO4', SET ION = 'SO4.P'),
OUT SD.P,
REPLACE$
/*Data is sorted for plotting of control charts
SORT SD.P,
BY TYP ION YEAR,
OUT SD.P,
REPLACE$
TEXT;
*** CONTROL CHARTS ARE BEING GENERATED ***
$
/*Control charts are plotted with NSD set to a max of 6 and min of -6
/*and output to file PLOTS.SD in 132 column format
PLOT SD.P (IF NSD > 6, SET NSD = 6)
(IF NSD < -6, SET NSD = -6),
BY TYP ION YEAR;
PLOT NSD * DECIMAL.DATE, TICKS Y -6 TO 6 BY 2,
GRID.LINES Y -2 TO 2 BY 2, LABEL X 'DATE SAMPLE WAS LOGGED INTO LABORATORY',
LABEL Y 'NUMBER OF STD DEV FROM THEORETICAL VALUE', EDGES T B L R,
PRINTER PLOTS.SD;
```

```
$
TEXT;
*** CONTROL CHARTS ARE FINISHED ***
$
CLOSE PLOTS.SD$
/*Data is sorted
SORT SD.P,
BY TYP ION MIX,
OUT CV.SORT
$
PURGE SD.P$
TEXT;
*** NOW COMPUTING PRECISION DATA ***
$
/*Counts number of determinations more than two and more than six
/*standard deviations from the theoretical value
AGGREGATE CV.SORT (KEEP TYP ION NSD)
(IF NSD>2 OR NSD<-2, GEN SD2=1)
(IF NSD>6 OR NSD<-6, GEN SD6=1),
COLLECT,
COUNT,
BY TYP ION,
OUT QA.COUNTS$
/*Percentages of the total are generated from numbers in AGGREGATE
MODIFY QA.COUNTS (RENAME n.SD2 = NUM.SD2)
(RENAME n.SD6 = NUM.SD6) (RENAME n.NSD = TOT.NUM)
(GEN PERCENT.OVER.2SD = NUM.SD2/TOT.NUM*100)
(GEN PERCENT.OVER.6SD = NUM.SD6/TOT.NUM*100),
OUT QA.COUNTS,
REPLACE$
/*Title for table 1 is prepared and data listed to file QA.COUNTS
TITLE T1 'TABLE 1: CONSTITUENTS IN RETRIEVAL WITH NUMBER OF DETERMINATIONS'$
TITLE T2 '*****************************************************************'$
TITLE T3 'TYP = data type: M=major, T=trace metal, N=nutrient, P=precip'$
TITLE T4 'TOT.NUM = total number of determinations'$
TITLE T5 'NUM.2SD = number > 2 standard deviations from theoretical  '$
TITLE T6 'NUM.6SD = number > 6 standard deviations from theoretical  '$
TITLE T7 'PERCENT.OVER.2SD = percent over 2 std dev from theoretical'$
TITLE T8 'PERCENT.OVER.6SD = percent over 6 std dev from theoretical'$
LIST QA.COUNTS, TITLE, PLACES 1, PRINTER QA.COUNTS
$
CLOSE QA.COUNTS$
PURGE QA.COUNTS$
TEXT;
*** DATA IS DELETED IF THE NUMBER OF STANDARD DEVIATIONS ***
*** IS GREATER THAN 6 FROM THE THEORETICAL VALUE ***
$
/*Determinations more than six std dev from mpv excluded
MODIFY CV.SORT (IF NSD > 6, EXCLUDE) (IF NSD < -6, EXCLUDE),
OUT CV.SORT,
REPLACE$
/*Statistical data generated by typ, ion
PERCENTILES CV.SORT (KEEP TYP ION MPV),
DES MPV.DES,
```

```
BY TYP ION
$
/*Range of theoretical concentrations determined
MODIFY MPV.DES (KEEP TYP ION LOW HIGH),
OUT MPV.DES,
REPLACE$
/*Title for table 2 and mpv data listed to file QA.MPV
TITLE T1 'TABLE 2: RANGE OF THEORETICAL CONCENTRATIONS (MPV) BY CONSTITUENT'$
TITLE T2 '************************************************************'$
TITLE T3 'TYP = data type: M=majors, T=trace metals, N=nutrients, P=precips'$
TITLE T4 'High and low values reported in milligrams per liter, except for '$
TITLE T5 'trace metals (T) and boron (B) reported in micrograms per liter. '$
TITLE T6 OFF $
LIST MPV.DES, TITLE, PRINTER QA.MPV
$
PURGE MPV.DES$
CLOSE QA.MPV$
/*Statistics generated by typ,ion,mix,mpv
PERCENTILES CV.SORT (KEEP TYP ION MIX MPV VAL),
DES CV.DES,
BY TYP ION MIX MPV
$
/*RSD is generated for precision data
MODIFY CV.DES (KEEP TYP ION MPV GOOD MEAN S.D.)
(GEN RSD=S.D./MEAN*100) (RENAME GOOD TO NUM) (RENAME MPV TO MPV.MIX),
OUT CV.DES,
REPLACE$
TEXT;
*** MORE COMPUTING ***
$
SORT CV.DES,
BY TYP ION MEAN,
OUT CV.DES,
REPLACE$
/*Title for table 3 and data is listed to file QA.CV
TITLE T1 'TABLE 3: PRECISION DATA BY DATA TYPE AND CONSTITUENT'$
TITLE T2 '************************************************'$
TITLE T3 'Table shows the NUM (number of determinations) for each ION and
TYP'$
TITLE T4 '(data type, M=major, T=trace metal, N=nutrient, P=precip) by
unknown'$
TITLE T5 '(MPV.MIX = theoretical value for the unique mix) with the MEAN, the
'$
TITLE T6 'S.D. (standard deviation), and the RSD (relative standard
deviation,'$
TITLE T7 'in percent) of the values reported by the laboratory.    '$
TITLE T8
'*****************************************************************'$
TITLE T9 'Values more than six std dev from theoretical are deleted'$
LIST CV.DES (IF NUM < 3, EXCLUDE), TITLE, PLACES 2, PRINTER QA.CV
$
CLOSE QA.CV$
PURGE CV.SORT$
TITLES RESET $
```

```
TEXT;
*****************************************************************************
               Preparing precision plots of the data

              WILL TAKE SEVERAL MINUTES FOR THIS STEP

    Disregard error messages - data is being placed in a plot file
*****************************************************************************
$
/*Macro to generate precision plots, RSD is set to max of 100,and
/*plots are output to file PLOTS.CV
MACRO PLOTS $
PLOT CV.DES (IF RSD>100, SET RSD=100)
(IF ION = 'XXXXXX', CONTINUE) (IF NUM < 3, EXCLUDE);
PLOT RSD*MEAN, EDGES T B L R, TITLES T2 CENTER
 '      ION = XXXXXX        TYPE = ZZ',
LABEL X 'MEAN CONCENTRATION OF REPORTED VALUES',
LABEL Y 'RELATIVE STANDARD DEVIATIONS, IN PERCENT', PRINTER PLOTS.CV;
$
MACEND$
/*Macro PLOTS is repeatedly called to generate precision plots.
/*Necessary to get unique axis scaling for mean values
RUN PLOTS, XXXXXX ALK, ZZ M $
RUN PLOTS, XXXXXX B, ZZ M $
RUN PLOTS, XXXXXX CA, ZZ M $
RUN PLOTS, XXXXXX CAAA, ZZ M $
RUN PLOTS, XXXXXX CL, ZZ M $
RUN PLOTS, XXXXXX ROE, ZZ M $
RUN PLOTS, XXXXXX F, ZZ M $
RUN PLOTS, XXXXXX MG, ZZ M $
RUN PLOTS, XXXXXX MGAA, ZZ M $
RUN PLOTS, XXXXXX K, ZZ M $
RUN PLOTS, XXXXXX SIO2, ZZ M $
RUN PLOTS, XXXXXX SICOL, ZZ M $
RUN PLOTS, XXXXXX NA, ZZ M $
RUN PLOTS, XXXXXX NAAA, ZZ M $
RUN PLOTS, XXXXXX SO4, ZZ M $
RUN PLOTS, XXXXXX NH4, ZZ N $
RUN PLOTS, XXXXXX KJD, ZZ N $
RUN PLOTS, XXXXXX NITR, ZZ N $
RUN PLOTS, XXXXXX NO2, ZZ N $
RUN PLOTS, XXXXXX P, ZZ N $
RUN PLOTS, XXXXXX PO4, ZZ N $
RUN PLOTS, XXXXXX CA.P, ZZ P $
RUN PLOTS, XXXXXX CL.P, ZZ P $
RUN PLOTS, XXXXXX F.P, ZZ P $
RUN PLOTS, XXXXXX K.P, ZZ P $
RUN PLOTS, XXXXXX MG.P, ZZ P $
RUN PLOTS, XXXXXX NH3, ZZ P $
RUN PLOTS, XXXXXX NO3, ZZ P $
RUN PLOTS, XXXXXX PO4.P, ZZ P $
RUN PLOTS, XXXXXX PHOS.P, ZZ P $
RUN PLOTS, XXXXXX NA.P, ZZ P $
RUN PLOTS, XXXXXX SO4.P, ZZ P $
```

```
RUN PLOTS, XXXXXX SPC, ZZ P $
RUN PLOTS, XXXXXX AL, ZZ T $
RUN PLOTS, XXXXXX SB, ZZ T $
RUN PLOTS, XXXXXX AS, ZZ T $
RUN PLOTS, XXXXXX BA, ZZ T $
RUN PLOTS, XXXXXX BAAA, ZZ T $
RUN PLOTS, XXXXXX BAT, ZZ T $
RUN PLOTS, XXXXXX BE, ZZ T $
RUN PLOTS, XXXXXX BET, ZZ T $
RUN PLOTS, XXXXXX CD, ZZ T $
RUN PLOTS, XXXXXX CDAA, ZZ T $
RUN PLOTS, XXXXXX CDT, ZZ T $
RUN PLOTS, XXXXXX CR, ZZ T $
RUN PLOTS, XXXXXX CRDCP, ZZ T $
RUN PLOTS, XXXXXX CRT, ZZ T $
RUN PLOTS, XXXXXX CO, ZZ T $
RUN PLOTS, XXXXXX COAA, ZZ T $
RUN PLOTS, XXXXXX COT, ZZ T $
RUN PLOTS, XXXXXX CU, ZZ T $
RUN PLOTS, XXXXXX CUAA, ZZ T $
RUN PLOTS, XXXXXX CUT, ZZ T $
RUN PLOTS, XXXXXX FE, ZZ T $
RUN PLOTS, XXXXXX FEAA, ZZ T $
RUN PLOTS, XXXXXX FET, ZZ T $
RUN PLOTS, XXXXXX PB, ZZ T $
RUN PLOTS, XXXXXX PBAA, ZZ T $
RUN PLOTS, XXXXXX PBT, ZZ T $
RUN PLOTS, XXXXXX LI, ZZ T $
RUN PLOTS, XXXXXX LIT, ZZ T $
RUN PLOTS, XXXXXX MN, ZZ T $
RUN PLOTS, XXXXXX MNAA, ZZ T $
RUN PLOTS, XXXXXX MNT, ZZ T $
RUN PLOTS, XXXXXX HG, ZZ T $
RUN PLOTS, XXXXXX MO, ZZ T $
RUN PLOTS, XXXXXX MOAA, ZZ T $
RUN PLOTS, XXXXXX NI, ZZ T $
RUN PLOTS, XXXXXX NIAA, ZZ T $
RUN PLOTS, XXXXXX NIT, ZZ T $
RUN PLOTS, XXXXXX SE, ZZ T $
RUN PLOTS, XXXXXX AG, ZZ T $
RUN PLOTS, XXXXXX AGAA, ZZ T $
RUN PLOTS, XXXXXX AGT, ZZ T $
RUN PLOTS, XXXXXX SR, ZZ T $
RUN PLOTS, XXXXXX V, ZZ T $
RUN PLOTS, XXXXXX VCOL, ZZ T $
RUN PLOTS, XXXXXX ZN, ZZ T $
RUN PLOTS, XXXXXX ZNAA, ZZ T $
RUN PLOTS, XXXXXX ZNT, ZZ T $
END$
/*Control is returned to USERPH.CPL to generate statistical report
/*and transfer it to the computer node designated by the user.
```

APPENDIX VII - LISTING OF COMPUTER CODES FOR USERPH.CPL

Program USERPH.CPL: command procedure language run by a phantom that generates statistical tables and plots using QA1.TRANS and transfers a final report to the office designated by the user.

```
&DEBUG &ECHO
OPEN T$0000 101 2
CLOSE T$0000
DELETE T$0000
term -xoff -FULL
A BQA>INFO.DIR
/*Causes the phantom to run at lowest priority
CHAP IDLE
&ARGS USERID
&ARGS NODE
&ARGS LAB
/*If cpl finds an error program goes to routine error_path
&SEVERITY &ERROR &ROUTINE ERROR_PATH
/*Routine to read userid, node, and labname and generate variables
&SET_VAR UREAD_UNIT := [OPEN_FILE USERID -MODE R OK]
&SET_VAR NREAD_UNIT := [OPEN_FILE NODE -MODE R OK]
&SET_VAR LREAD_UNIT := [OPEN_FILE LABNAME -MODE R OK]
&SET_VAR USERID := [READ_FILE %UREAD_UNIT% OK]
&SET_VAR NODE := [READ_FILE %NREAD_UNIT% OK]
&SET_VAR LAB := [READ_FILE %LREAD_UNIT% OK]
CLOSE (USERID NODE LABNAME)
DELETE (USERID NODE LABNAME)
COMO BQA>INFO.DIR>PH.%USERID%.COMO
/*Data output from INFO is edited to be compatible with PSTAT
&DATA ED QADNSP
BRIEF
TOP
L \;C/\/ /G;*
FILE SD.DATA
Q
&END
DELETE QADNSP
/*Copy of retrieval is saved
COPY SD.DATA BQA>USER.DIR>%USERID%.QADATA.[DATE -FTAG]
/*Pstat software is invoked in batch mode with transfer file QA1.TRANS
&DATA PSTAT -BATCH QA1.TRANS -OUT BATCH.COMO
&END
COMO -E
COMO BQA>INFO.DIR>PHA.%USERID%.COMO
/*File PLOTS.CV is edited for unnecessary text
&DATA ED PLOTS.CV
BRIEF
LOC There;DELETE;*
FILE
&TTY
&END
/*Final statistical report is generated from files output from PSTAT
/*Header.nwql contains an explanation of report output for the NWQL;
```

```
/*while the other files were output from PSTAT
&IF %LAB% = OCALA &THEN &GOTO OCALA_ROUTINE
&DATA CONCAT QAPLOTS -OVE -NHE
HEADER.NWQL
QA.COUNTS
QA.MPV
PLOTS.SD
QA.CV
PLOTS.CV

QUIT
&END
&GOTO NWQL_NEXT
&LABEL OCALA_ROUTINE
/*Header.ocala contains an explanation of report output for the
/*Ocala WQSU report.
&DATA CONCAT QAPLOTS -OVE -NHE
HEADER.OCALA
QA.COUNTS
QA.MPV
PLOTS.SD
QA.CV
PLOTS.CV

QUIT
&END
&LABEL NWQL_NEXT
/*Report file is edited to inform printer of Fortran form feeds
&DATA ED QAPLOTS -OVE -NHE
I ^001^001
FILE
&TTY
&END
DELETE (QA.COUNTS QA.MPV PLOTS.SD QA.CV PLOTS.CV SD.DATA)
/*Report file is tagged with userid
CN QAPLOTS QAPLOTS.%USERID%
/*Report is transferred to computer node designated by user
&DATA FTR QAPLOTS.%USERID% FTS_DEPOT>QAPLOTS.%USERID%.[DATE -FTAG] -DS
%NODE%~
 -LOG BQA>USER.DIR>USER.LOG -NQ
&END
/*Copy of report is saved tagged with userid, date, time
COPY QAPLOTS.%USERID% BQA>USER.DIR>%USERID%.QAPLOTS.[DATE -FTAG]
DELETE QAPLOTS.%USERID%
DELETE BQA>CHECK.COMO
COMO -E
&RETURN
/*Error routine so program crashes softly if cpl error is found
/*File check.como is deleted so other users are not locked out
&ROUTINE ERROR_PATH
COMO BQA>PHERROR.COMO
DATE
TYPE
TYPE There was a problem with the retrieved dataset and no output will
```

```
TYPE be generated.
TYPE .
LD
DELETE (BQA>CHECK.COMO BQA>INFO.DIR>SD.DATA)
COMO -E
&RETURN
```


*U.S. GOVERNMENT PRINTING OFFICE: 1990-0-773-204/20016