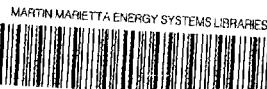


ornl

OAK RIDGE
NATIONAL
LABORATORY

MARTIN MARIETTA

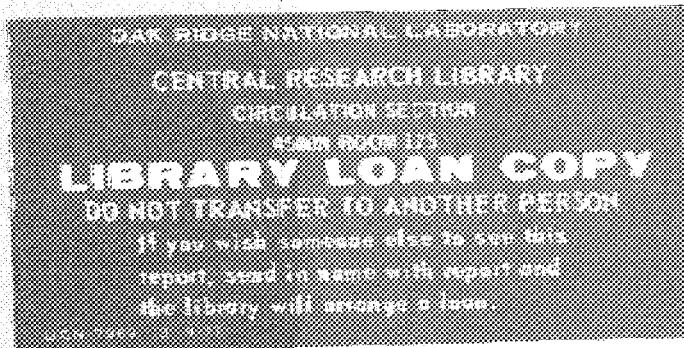
ORNL/TM-11540



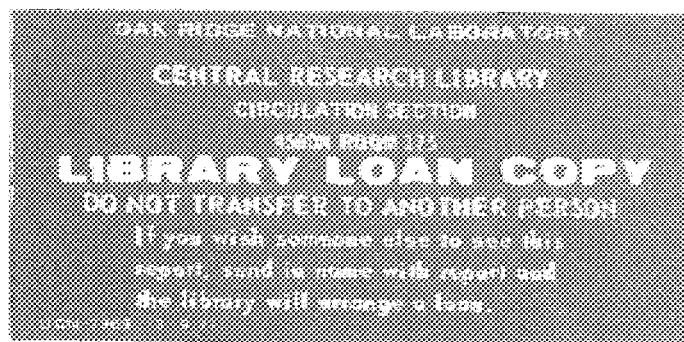
3 4456 0315421 7

Program for Preparing Output Data
from a Flow Injection Spectrometer
for Entry into Analis Data Base of the
Analytical Chemistry Division
Oak Ridge National Laboratory

T. R. Mueller



May 1990



OPERATED BY
MARTIN MARIETTA ENERGY SYSTEMS, INC
FOR THE UNITED STATES
DEPARTMENT OF ENERGY

This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from the Office of Scientific and Technical Information, P.O. Box 62, Oak Ridge, TN 37831; prices available from (615) 576-8401, FTS 626-8401.

Available to the public from the National Technical Information Service, U.S. Department of Commerce, 5285 Port Royal Rd., Springfield, VA 22161.

NTIS price codes—Printed Copy: ACS Microfiche A01

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Prepared by the
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

Published by
Martin Marietta Energy Systems, Inc.
for the
U.S. DEPARTMENT OF ENERGY
under Contract No. DE-AC05-84OR21400

ORNL/TM-11540

PROGRAM FOR PREPARING OUTPUT DATA FROM
A FLOW INJECTION SPECTROMETER FOR
ENTRY INTO AnaLis DATA BASE OF THE
ANALYTICAL CHEMISTRY DIVISION
OAK RIDGE NATIONAL LABORATORY

T. R. Mueller

May, 1990

Prepared by the
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831-6127
operated by
MARTIN MARIETTA ENERGY SYSTEMS, INC.
for the
DEPARTMENT OF ENERGY
under contract DE-AC05-84OR21400

MARTIN MARIETTA ENERGY SYSTEMS LIBRARIES



3 4456 0315421 7

CONTENTS

1.	OVERVIEW.....	1
2.	PROGRAM SOURCE CODE	1
3.	EXECUTION OF THE PROGRAM.....	2
4.	CONCLUSIONS AND POSSIBILITIES FOR FUTURE DEVELOPMENT... .	5
5.	INSTRUCTIONS TO THE USER	6
6.	QUALITY ASSURANCE COMPLIANCE.....	11
7.	INSTRUCTIONS FOR CODING BY THE FIS OPERATOR.....	13
8.	REFERENCES.....	15
Appendix A.	PART I. PROGRAM SOURCE CODE LISTING PART II. LOGICAL FLOW OF THE PROGRAM	
Appendix B.	SAMPLE DATA REPORT FROM FIS	
Appendix C.	RUN-TIME DIALOG	
Appendix D.	SAMPLE OF DATA AFTER FORMATTING BY FIS_PARSE	

1. OVERVIEW

- 1.1 The Analytical Chemistry Division (ACD) is attempting to improve the quality of data taken from instruments, recorded, and stored in its data base. One avenue for realizing this goal is to reduce the manipulation of data by hand operations. This report describes the design and implementation of a program, FIS_PARSE, that processes output from a Lachat, Inc., flow injection optical spectrometer(FIS) and prepares it for storage in the Analytical Chemistry Division's data base, AnaLis; therefore, provision is made for transmittal of both raw data and selected results to archives. It is necessary to review the data before transmitting them to the data base; therefore, direct transfer of results from the computer used to operate the spectrometer was not selected as the method of choice.
- 1.2 The raw data may be written in ASCII format to a floppy disc or sent directly to a storage file on the ACD VAX computer. The data can then be listed and inspected at any work station equipped to read the data. The ACD has its own VAX-8300 (Product of Digital Equipment Corp.) computer that is connected into a network accessible from numerous points in the ACD environment. If the work station is connected to this system, data may be transferred from the floppy disc to the VAX for processing.
- 1.3 FIS_PARSE is an interactive program. The user is offered a number of processing options that ultimately allow a customer-specific report to be delivered to AnaLis. This latter feature allows customers to obtain their results by direct (electronic) access to AnaLis file data.
- 1.4 Some familiarity with the operation of a PC running under IBM-or MS-DOS is required for use of the program. It is also assumed that the operator is conversant with the requirements for data that are to be reported for flow injection optical spectrometry and is in a position to identify and select data that qualify for inclusion in AnaLis.

2. PROGRAM SOURCE CODE

- 2.1 A listing of the program is included as Appendix A. Part I. Logical flow of the program during execution forms Part II of Appendix A. Appendix B. shows how the report from the spectrometer appears before processing. Examples of run-time dialogs and output during execution are included in Appendix C. Appendix D is included to show the format of the data prior to transmittal to AnaLis.
- 2.2 Only one subroutine is included in the program; namely, a routine to read a line of the primary report from the flow-injection spectrometer (FIS). Program flow is from 'top-to-bottom' and should present little difficulty in associating the program source code and the logical flow of Part II. There is some redundancy in parts of the program, but it was felt that maintenance would be simplified by using this approach.

- 2.3 The program, FIS_PARSE.FOR is written to run on the Analytical Chemistry Division's VAX-8300 computer(Digital Equipment Corp.). Since AnaLis is also accessed via this computer and since all files reside in the same environment, communication is simplified. The long variable names permitted in FORTRAN-77 facilitates 'self-documentation'.

3. EXECUTION OF THE PROGRAM

- 3.1 FIS_PARSE first addresses itself to the problem of reading and formatting the report from the FIS. Figure 1 is a reproduction of the report for one tray of samples. Figure 2 shows the appearance of the report when two species are analyzed and reported simultaneously. The FIS instrument has the capability of performing the analysis and reporting of four species simultaneously. Although the instrument is not normally used in the four-channel mode, the program is written to accommodate this eventuality.

- 3.2 The report from the FIS is treated by FIS_PARSE as if it consists in 'header' and 'results' areas. The header is that portion of the report before Cup 1. Results are found below that point. There may be entries for as many as 40 samples/tray.

- 3.3 Each line of the report contains 60 characters. A new tray is signaled by the header line starting with,"QuikCalc...". The program reads the following information from the header:

- 1- Date and time of analysis
- 2- Reference (Used as 'sequence number')
- 3- Method identification
- 4- Operator identification
- 5- Tray Comments. This field contains what are referred to as 'customer request numbers'. These numbers identify the owner of the samples and are used to customize reports.
- 6- The Analyte(s) present
- 7- The units in which the results are reported

- 3.4 The only data from this area required for AnaLis are the operator's identification, the method name, and the units of measurement. The other information is used by FIS_PARSE to identify the results.

- 3.5 After the header is read, the operator is queried for processing instructions that apply to the entire tray:

- 1- Skip processing of the tray?
- 2- Select Request numbers to process or delete
- 3- In the case there are multiple analytes, select those to process.

If the operator is satisfied with the choices made, processing proceeds to the 'result' area.

3.6 A 'result' line contains the following information:

- 1- Cup # (1 to 40)
- 2- Sample identification(ID)
- 3- One to four columns of analytical results
- 4- The dilution factor
- 5- Weight of sample, if applicable

The 'results' lines are all read and stored on a first pass. The number of samples on the tray are also determined in this pass. The stored lines are then recalled sequentially and each line processed for the desired data. Pre-arranged coding of the sample ID permits the program to identify several types of data. Lines which do not contain sample results begin with a letter of the alphabet; lines containing sample results must begin with a numeral.

3.7 During the first pass, reagent blanks are flagged with respect to their positions on the tray. If more than one blank is detected during this pass, the values of the blanks are displayed with the average. The blanks for each analyte are presented separately. Four options are given the operator:

- 1- Select one of the values
- 2- Select the mean value
- 3- Delete, one at a time, and recalculate the new mean
- 4- Enter a number for the blank

In subsequent processing, the operator can choose whether to subtract the blank or not. Blanks are first corrected for conversion to species other than the element. If the blank is subtracted, the result is checked to determine if it is below the detection limit.

3.8 The unjustified columnar results present a slight difficulty in reading the data. The free-form format used in producing the original report form (see Figure 1) allows staggered columns; i.e., column spacing is relative rather than absolute. The fields do not actually overlap, but the program must correctly find the decimal point and then right-justify the characters so that they can be converted to the correct real number. Another difficulty is that non-numeric character results used when reporting that the results are below the detection limit (reported as < x.xx) or high (reported as high or HIGH) are not convertible into real numbers. The alphabetic characters must, therefore, be stripped before any arithmetic operations are attempted.

3.9 As the columnar data are processed, high results are called to the operator's attention, then eliminated from the data reported to AnaLis. Such samples would normally be diluted and another analysis performed on the diluted material. A real number is required for comparison purposes if reagent blanks are subtracted from the reported results.

3.10 The results on the original report already incorporate the necessary corrections for dilution and sample weight. Data for dilution factors and original sample weights are not needed except for their use in assessing the necessity for making blank corrections.

3.11 Sample 'type' numbers are assigned to each coded sample type. Although only actual (customer-submitted) samples are presently processed by this program for inclusion in AnaLis, results for any sample type could be stored in a permanent record. Actual samples are given the code '1' and reagent blanks are '4', for example. Type '7' is assigned to non-coded entries. A tally of the numbers of each sample type identified is kept and reported to the operator at the end of the review/submission session. The complete list of sample types is found in FIS_PARSE, Appendix A.

3.12 Sample Numbers

- 3.12.1 The sample number is the unique signature by which a sample and its corresponding analytical result are associated. Except for missing leading zero's in the index number, no attempt is made to correct an incorrectly formatted sample number. If the sample number cannot be interpreted by FIS_PARSE, the operator is given the opportunity to insert the correct one.
- 3.12.2 All ACD sample numbers are of the type 'yymmdd-sub', where 'yy' is the last two digits of the year, 'mm' is the month, 'dd' is the day, the dash is a separator, and 'sub' is the index or sub-sample number. The first six digits plus the dash are referred to as the 'root' sample number. This is the only form that AnaLis will accept(10 characters). The leading zero(s) on the index number will be supplied if missing. This is the only acceptable corruption of the sample number permitted by FIS_PARSE. It would be more correct for operators to enter the totally correct sample number;however, the Lachat program sequences the numbering automatically, and this approach is probably prone to the introduction of fewer errors.
- 3.12.3 As an input line is scanned for data, the appearance of the '-' in the seventh position of the root sample number is taken as an indication that a new customer request is being processed. If the root and the index are both valid, the root is stored. A flag is set to mark this fact while the rest of the line is searched. At this point in the processing the operator is given the opportunity to enter instructions for the subsequent processing of the samples submitted with the specific request number. If the result found is valid, the flag is cleared.

3.13 Tailoring Results to Customer Specifications

The following types of customizing have been provided:

- 3.13.1 If no detection limit for the analysis is resident, enter the detection limit.
- 3.13.2 All results from the FIS are reported for the element. Some customers may prefer to have nitrogen reported as nitrate or nitric acid--phosphorous as phosphoric acid or the pentoxide. Frequently selected options have been included in the program as menu options. Others could be added easily. If the species reported is not the element, the appropriate correction factor is applied when the result is processed. The operator is queried for the name of the analysis to be reported to the customer. Default names are automatically inserted in the prompts.

3.13.3 Identification of procedures. There are two procedure numbers associated with a sample result--the preparation procedure and the analysis procedure. The operator selects whether to include these or not. If either or both are to be entered, the operator is prompted for their entry at the appropriate time.

3.13.4 Subtract the reagent blank.

A list of options selected is next displayed. If the operator is satisfied with the choices, the program proceeds with the processing of the result area.

- 3.14 As each line is read and processed, the results are displayed on the monitor. Appendix B is a record of a review/submission session. If different from the original result, or a conversion factor changed the absolute value of the detection limit, the new detection limit is displayed, followed by the original data. The next two lines are data to be stored. Two flags are also displayed. An '*' denotes no change from the original input data. If a conversion factor has been applied, a 'C' is displayed. If a blank was subtracted, the '*' or 'C' is followed by a '-B'. The cup # terminates the displayed line.
- 3.15 Since there is a finite time required for processing the data and transmitting the returned results, the operator has enough time to interrupt the processing with the 'HOLD' key on the keyboard of the computer to examine the data. Processing is resumed with a second stroke of the 'HOLD' key.
- 3.16 A sequential data file,FILE_TRANSFER, is created at the beginning of the session. The file is opened with the 'status unknown' argument, so that, if no file exists in the directory, one is created. If a file does exist, it is overwritten by the new data. Parallel files,TEMPO1.DAT, are also created so that the operator can examine archive files. These files are created with the 'status new' argument, which creates a new file for each session. Some attention must be given to the number of these files that are resident in the directory. The 'PURGE' command to the VAX will delete unwanted files.

4. CONCLUSIONS AND POSSIBILITIES FOR FUTURE DEVELOPMENT

- 4.1 FIS_PARSE has been in use since May, 1988. As originally written, it processed only one analyte per tray. Soon after its inaugural, work commenced to accommodate the maximum, four-channel capability of the Lachat, Inc., FIS. The version described in this document has been in use since September 20, 1988. Intermediate versions produced the same 'results' entries, but were tailored to different reporting requirements.
- 4.2 While this program was written for a specific application, the approach taken in programming is quite general. The program reads a 'line' of an ASCII file, searches it for a field of interest, extracts that field, formats it according to an established set of rules and stores the results on the desired medium.

- 4.3 Much of the dialog between operator and computer could be implemented more attractively with a form management program. This approach could lead to still more accurate input of data, since default fields would appear in context and fields to be filled in by the operator would show the input requirements without recourse to format explanations that could be subject to misinterpretation.
- 4.4 Deliberate attempts to confuse the program have been made by inserting incorrect responses to queries by the computer. It appears that the program recovers correctly and logically under these circumstances. However, the program cannot distinguish errors in values entered by the operator. Very little is required from the operator that could not be found in a data file and read into FIS_PARSE when needed. Once these supplementary files are created and proofed, there should be little chance of corrupting results by hand insertion of data.

5. INSTRUCTIONS TO THE USER

- 5.1 This section contains instructions for the use of FIS_PARSE. Please read through it before trying to send data to the VAX. Please make notes while running it, so that the dialog can be made more meaningful in subsequent versions.
- 5.2 Prepare, starting with a freshly formatted or re-formatted disc, a disc to be used to get a listing of the files to be transferred to the VAX. The operator of the FIS will prepare the transfer disc containing files from the spectrometer in ASCII format. These files will have names such as, 8805010a.rpt. The only requirement for the format of these names, as far the subsequent copying routine is concerned, is that they all have the extension, '.rpt'.
- 5.3 In the following section you type the underscored entries. The '#' sign means a space is required. There are other ways in which the files may be transferred. The ultimate goal is to produce a file on the VAX with the results of one or more files from the FIS.

Place the prepared disc in drive a of your computer or terminal.

In DOS, make your directory 'a:'

At the DOS prompt,'a:>' copy#*.rpt#fis.dat

When done, log on to the VAX using the terminal emulator, Smarterm 240 (Persoft, Inc.)

The following steps create a file called 'fis.dat' on the VAX:

\$ create#fis.dat<CR> <CR> means to hit the ENTER key

<alt>T

This invokes the TRANSMIT mode of Smarterm (Communication Program, Persoft, Inc.), and will copy files on your disc to the VAX. The cursor points to the 'filename' area. If the cursor does not point to the filename area, type 'F'.

Type, a:fis.dat<CR> for the filename.

At the prompt, type <CR>; transmission should begin.

At the end of transmission the message END OF TRANSMISSION will appear (in red field). Follow instructions, hit a key.

Type, <alt>T to end the transmit mode

\$ <cntl>Z to close file on VAX--important!

- 5.4 There is now a file called 'fis.dat' on the VAX. You are ready to run fis_parse.

\$ run#fis_parse<CR>

- 5.5 Answer questions asked by program; the first question will ask for the filename to read. You hit ENTER to use the default name, 'fis.dat'. If you want to use another file, perhaps an earlier version of fis.dat, enter fis.dat;version, where version is the number of the version you want to process (for example,fis.dat;6).

- 5.6 The program will ask for other processing instructions as well as locate missing or incorrectly entered information. Reference to Appendix C. will be helpful in visualizing the ensuing dialogue.

- 5.7 The badge number identifies the operator of the FIS. No processing can take place without a proper badge number. If there is no badge number, the program will ask for one to be entered. If requested, enter the correct badge number. Badge numbers shorter than five (5) digits should be preceded by a zero (0).

- 5.8 The program reads the header portion of the first data file from the FIS. The method of analysis, the date and time of the analysis, and the sequence number is displayed. Next, a list of the Request Numbers and their total is displayed.

- 5.9 You are then asked if you want to process this tray of samples. You hit ENTER if you do, a \$<CR> if you want to skip the tray.

- 5.10 If more than one analyte is found on the tray, you will be given the opportunity to select which analyte(s) to report. If you hit ENTER, all data will be reported. Follow the instructions on the screen.

- 5.11 You now have the option of selecting or deleting some or all of the samples for given Request Numbers. If you want to report all of the samples, you hit ENTER. If you want to select those request numbers for which samples are to be reported or those for which samples should not be reported you type a \$<CR>. The format for entering request numbers is displayed. Follow instructions on the display screen. If you enter incorrect request numbers the program will ask again if you want to process data by request number. You may then elect to report all (ENTER) or enter \$<CR>.

- 5.12 When you have entered acceptable request numbers or bypassed that step, the program asks if you are ready to process the file. If you are, hit ENTER; if not, type anything else and you will return to the first question and be given the opportunity to change processing instructions.
- 5.13 If you typed ENTER, the program reads and displays the data report section of the file. You may use the 'HOLD' or 'SCROLL LOCK'(or cntl-S) to interrupt processing if you want to examine the data being read. When the data have been read and stored, you will be prompted for the detection limit for the analyte reported in column 1 of the results if there is no reagent blank or fewer than two on the tray. Enter the limit for the element, if different from the displayed default value.
- 5.14 If more than one reagent blank is found, you will be asked what value the program should use for the reagent blank. Four options exist: 1) Select one of the values, 2) use the mean value, 3) enter a value from the keyboard, or 4) delete one or more of the results. If several blanks were found, you may delete selected ones. The program recalculates the mean for the ones not deleted, and you may elect to choose that value. Follow the instructions on the screen to make your selections of the blank value to use.
- 5.15 Each line of data corresponds to a vial on the sample tray. The program once more reads through its stored data file and displays what is found until it encounters the first data which corresponds to the format for a sample number. Remember that this is six digits, a dash, and three sub-sample digits--ten characters in all. The presence of the dash signals the program to look for a new request number.
- 5.16 When a new request number is found, you are given an opportunity to customize the report to meet the demands of a specific customer. The Request Number is displayed. You are then asked for a detection limit that may be higher than the detection limit for the method. Enter a number or, if you hit ENTER, the detection limit for the method will be assumed.
- 5.17 You are next asked whether or not to delete specific results. Type 'y' if you want to select results to delete; hit ENTER to report all results.
- 5.18 The program recognizes codes for methods and analytes. If the sample is a nitrogen-containing species, questions will relate to nitrogen,nitrates, or ammonia. If the sample is a phosphorous-containing species, questions pertaining to how to report phosphorous will be asked.
- 5.19 The original data from the FIS is reported as either 'N' for nitrogen or 'P' for phosphorous. Customers may want their report in terms of other species. You may select from a menu certain common species for N or P conversions. If you select from the menu, the gravimetric factors will be applied automatically and a default name supplied.
- 5.20 You are then asked to supply the name by which AnaLis will recognize the report. If you have selected an entry from the menu, the default name displayed may be the one you want to use; if not, you may enter the correct name.

- 5.21 In addition to the sample number, there are two other numbers associated with a sample, the preparation number and the analysis number. At present there is no way to enter these from a file. You must supply them if they are to be entered. You can force them to be changed by requesting that they be changed at this point in the dialog. If you do not change them and they are not found when needed, the program will ask for them. Their input is optional; that is, you may hit ENTER to leave them blank or enter numbers for one or both.
- 5.22 A summary of your responses and default values is then displayed. You should examine this display to determine if the correct selections have been made. If you are satisfied with the values shown, hit ENTER; otherwise, type any letter and you will have the opportunity to re-enter your choices.
- 5.23 If a value for a reagent blank exists (see para N), you will be asked whether to subtract it from samples or not. If you elect to subtract it, enter a 'c'; if you do not want to subtract it, hit ENTER.
- 5.24 If you have hit ENTER, the program now has all the information it needs to process the data. The program reads all lines beginning with a number as if the rest of the line contained a real sample number and data. If the recovered line is not blank and the program cannot find a valid sample number (yymmddsss), it will query you for the correct sample number. If the entry really is a valid sample, correct the number according to the above format; if not, you may delete it by entering 'd'. The format for a real sample number is, e.g., 880501-123. That is, six numbers, a dash, and three digits which represent the sub-sample.
- 5.25 If the program finds a dash in the seventh position, it assumes that a new request number is to be processed. The line being read must contain a valid sample number in the first ten positions, but it may be followed by '+' or 'd'. The '+' indicates a spiked sample, the 'd', a duplicate.
- 5.26 There is one exception to the above rules. The sub-sample number need not contain three digits. The program will supply leading zero's to complete the required three digits.
- 5.27 At present, spiked samples are ignored; duplicates are reported. If duplicates are not to be reported, you can delete them in AnaLis editing.
- 5.28 See the FIS operator instructions in Section VII. for coding of standards and other 'special' samples.
- 5.29 When no more data is found in the fis.dat file, the program ends, returning control to the VAX monitor and the \$ is displayed. The program types a message to the operator that contains a list of material types found on the tray and the number of each type found. This list can be expanded to meet any needs of the operator(editor). Implied is the fact that, once identified, any of these data types can be stored in a file for future reference. Finally, the version of FIS_PARSE used to prepare the transfer file is listed.

- 5.30 The edited data are now in a file 'file_transfer.dat'. You transfer this file to AnaLis by typing '@file_data<CR>'. After transferring to AnaLis, FILE_TRANSFER.DAT is deleted from the disc.
- 5.31 FIS_PARSE also prepares a file called 'TEMPO1.DAT'. This file is identical with FILE_TRANSFER.DAT, except that it remains on the disc after FILE_TRANSFER.DAT has been dumped to AnaLis.
- 5.32 You will need to 'purge' TEMPO1.DAT occasionally or your disc will fill with these files.

To purge, you enter the following at the '\$' prompt of the VAX:

\$ PURGE#tempo1.dat<CR>

The last file prepared will remain on the disc. The TEMPO1.DAT files provide a way to check what has been processed by FIS_PARSE.

- 5.33 After you have prepared 'FILE_TRANSFER.DAT' you may want to look at what you have stored in that file before sending the file to AnaLis. To get a listing of the file do the following:

At the VAX prompt, type

\$ run#fis_read<cr> (fis_read)

The program will request that you select the file to read. The default is FILE_TRANSFER.DAT. You may instead request to read one of the TEMPO1.DAT files. To do this type :

\$ tempo1.dat;version<CR>

where 'version' is the number of the version to read.

After the last entry, three dollar signs,'\$\$\$', should appear to indicate that FIS_PARSE terminated correctly. If the \$\$'s are not present, AnaLis cannot interpret the data in the file. One way this can happen is that you stopped processing with FIS_PARSE by using 'CNTL-C' or some other means to quit before the end of the prepared file was found by FIS_PARSE.

6. QUALITY ASSURANCE COMPLIANCE

- 6.1 This section of the report sets out criteria for determining the quality of the data inserted into the AnaLis data base as a result of computer transfer and processing of data from the FIS and the means by which such assessments might be accomplished. It should be noted that this report does not address itself to the quality of the preparation or measurement methods used to obtain the original data; such information is found with the methods. This report is limited to those procedures which are applied to the results after the primary data record is transferred to either a floppy disc or to the host computer.
- 6.1.1 The quality of the results may be assessed by examining dialog between an operator using the program and the computer as recorded by a run-time log of the dialog. An example of such a dialog is presented in Appendix C. Insertions by the operator are underlined; otherwise, all text is generated by the computer. No operator symbol is visible where a query by the computer was answered with the default option.
- 6.1.2 It can be seen in a perusal of Appendix C. that very little operator input is required in order to process a large amount of data. Thus one goal, that of minimizing the amount of data entered by an operator or analyst, has been accomplished. It remains to show that 1) all necessary information has been extracted from the primary report(test by running FIS_READ), 2) that, where processing of the primary data is required, the results of calculations are correct(see hand calculations as notes in Appendix C.), and 3) that the correct data have been entered into AnaLis (verify by examining data in AnaLis).
- 6.1.3 Ancillary data required for processing was taken from sources identified in the Reference Section of this report. A key to the documentary comments inserted into Appendix C. is listed with the references.
- 6.1.4 Several ASTM Standards were consulted for guidelines in preparation of this report. Other QA procedures were also used as guides. These are listed with the References.
- 6.1.5 At the time of writing of this report, the author of the program is serving as custodian. All changes should be cleared with the author. It shall be the custodian's responsibility to document changes and to establish the impact these may have on the quality of previously reported results. Archival copies of all programs and their periods of use shall be maintained and documented. Source code for programs that require protection should have attributes that prevent unauthorized changes.
- 6.1.6 Maintenance of the program shall terminate if the method passes out of use.

- 6.2 FIS_PARSE identifies a tray of samples when it finds the report title, 'QuikCalc...', properly positioned on a line. Termination of the program occurs when there are no more lines of valid data or the title does not appear after the program reads several empty lines. Thus, the results of any number of trays of samples may appear in one file of data from the FIS. The number of trays of samples processed is reported at the end of a session.
- 6.3 The number of vials on a tray are counted during the first pass through the 'results' section of the primary report. The total number of vials for the entire file processed is reported at the end of the session. If the operator of the FIS has complied with coding requirements for the contents of each vial on a tray, FIS_PARSE can identify any type of sample.
The sums for every type of sample vial identified (blanks, standards, etc.) are reported at the end of the session. Also reported are the total number of unidentified sample vials.
- 6.4 If a result for a vial containing a sample is above the acceptable range, the FIS primary report contains the word 'high'. Processing is suspended when a high result is found so that the operator can mark that vial for dilution or other treatment and re-measurement. These vials are also counted and the number of high results reported at the end of the session.
- 6.5 For various reasons, it may be desirable not to report results for individual samples. These results could be removed by editing the primary data file. However, the possibility of corrupting a file always exists when using an editor. It is preferable to delete results during the FIS_PARSE session. A record of the number and analyte type for all deletions is reported at the end of a session.
- 6.6 It is necessary occasionally to modify the processing program, FIS_PARSE. From a QA perspective, it is necessary to identify the version of FIS_PARSE used during a processing session. The version of FIS_PARSE used is reported at the end of the session. At the present time there is no convenient way to assure that the data in AnaLis were entered via a particular version of a program. Provision for automatic inclusion of this information in AnaLis would improve the traceability of results.
- 6.7 Information implied by the underscores in paragraphs B.through F. is all displayed on one screen for the operator's inspection. A hard record of this information can be obtained by printing the screen on a local printer. The printed copy can be filed with other documentation.
- 6.8 With a copy of a run-time dialog similar to that of Appendix C. in hand, an auditor can verify each step of the processing by FIS_PARSE. Finally, the user or auditor can display or print the results about to be transferred to AnaLis by 'typing' the file, FILE_TRANSFER.DAT. Alternatively, a program has been written to simply read and display the data in this file with identifiers for each line of data. Such a listing is included in this report as Appendix D. After transfer to AnaLis, the data may be viewed with AnaLis procedures.

7. INSTRUCTIONS FOR CODING BY THE FIS OPERATOR

- 7.1 In order that FIS_PARSE can extract the correct information from the files prepared by the FIS, it is necessary to adhere to a rigid coding and data formatting scheme. This section of the report gives details of the coding required.
- 7.2 Operator identification is via a 6-digit number. At least five digits must be specified. For shorter badge numbers, a leading '0' should be inserted. Entry of initials instead of a badge number will be trapped during the running of FIS_PARSE, resulting in operator inconvenience and delays.
- 7.3 The Sequence Number, or Reference Number has the following format: ymmddxx, where xx is the daily sequence number. It should be serially numbered starting with 0a,0b,... (or 0A).
- 7.4 The sample identification field is used to identify types of materials in the vials. The following coding will be used:

If the first character is

H or h water blank
S or s standard
E or e EPA material (standard)
B or b reagent blank
P or p Pet
0 - 9 Sample

Anything else will be reported as 'unknown'.

If the last character is

+	Spiked sample
d	Duplicate sample

- 7.5 The area of the report reserved for comments will be used to transmit the Customer Request Numbers. These will be entered contiguously with the semi-colon (;) used as a separator. The lab identifier will not be included; e.g., 'EAL' is not included. Thus, if samples from two requests were included on one tray of samples, and the request numbers were EAL9876 and EAL12345, the tray comment area would contain the entry: 9876;12345. The comment area has room for 40 entries. FIS_PARSE associates the first group of samples with the first request number, the second group with the second, etc.

7.6 Sample numbers will be entered as follows:

881009-123 To correspond exactly to the sample number of record for the
24 specific sample.
137 The sample number 881009-024 will be synthesized
by FIS_PARSE.
. 24 and 137, etc., are sub-samples for purposes
of coding.

880929-64 Indicates the beginning of a new customer request

7.7 Changes in coding practice or the introduction of new codes must be cleared with the custodian of FIS_PARSE. Source code for programs that require protection should have attributes that prevent unauthorized changes.

8. REFERENCES

- A. Gravimetric factors for conversion of nitrogen and phosphorous to other than elemental species were taken from The Handbook of Chemistry and Physics, The Chemical Rubber Co., Cleveland, Ohio, 53rd ed., 1972.
- B. Atomic Weights were taken from the source quoted in A.
- C. ASTM Standard E 622-84, Standard Generic Guide for Computerized Systems.
- D. ASTM Standard E 627-82, Guide for Documenting Computerized Laboratory Systems.
- E. Consideration was also given to proposed guidelines for quality assurance in a draft of ANSI/ASME NQA-3, Rev. 1.
- F. AC-OP-000-0502, Writing and Issuing a Procedure, Draft 2, dated May 24, 1989, P. L. Howell.

THIS PAGE LEFT BLANK INTENTIONALLY

APPENDIX A

PART I. PROGRAM SOURCE CODE LISTING

This appendix is a listing of the program, FIS_PARSE.FOR, used to parse the output from a flow injection spectrophotometer. Data are prepared in format compatible with the data base, Analis.

```
1      program fis_parse
2      ! Written 3/30/88 by T.R.Mueller
3      ! Version 8/30/88 Re-written for multi-channel procedures
4      ! Version 9/15/88 For deleting selected species for samples and
5      !           corrected to pick up request #'s on multiple
6      !           lines and display 4-to-the line.
7      ! Version 9/20/88 To correctly capture short sub-sample #'s with
8      !           trailing 'd'(duplicate).
9      !           To find badge # when 'Method' causes displacement
10     !           of normal field position for "Operator".
11     ! Program to decode output from flow injection spectrometer and
12     !           format data for entry into Analis<via 'file_transfer.dat'>.
13     ! FORTRAN-77 for the VAX
14
15     ! Standards and blanks have been decoded and counted, but not stored
16
17     ! Format of data from FIS:
18
19     ! Line 1 - QuikCalc...starts in col 19
20     !   2 - Date and time      col 34
21     !   3 - Tray ID          col 44-52, Sequence Number
22     !   4 - Method (25 characters) col 9 ; Operator badge # col 34
23     !   5 - blank
24     !   6 - Tray comments--Used for Request #'s;req #'s terminated by ';'
25     !   7 - blank
26     !   8 - Analyte: iteration of method(s) on line 4. col 6
27     !   9 - Base correction, not used
28     !  10 - technique, not used
29     !  11 - blank
30     !  12 - 15 not used
31     !  16 - blank
32     !  17 - Analyte. This line read to determine # of species reported
33     !  18 - Cup, Sample ID,measurement units,dilution factor (4 cols to read)
34     !  19 - blank
35     !  20 - First line containing sample report
36     !       Cup #      col 1-3
37     !       Sample ID    col 5-15
38     !       data and detection limit info. Can start in col 16
39
40     character *128  req_del
41     character*60   filler,blanks,fill_buf(42)
42
43     character*10   sample_number,c_sample_number
44
45     character*30   method,method_code,analysis,a_method_code
46     character*30   t_method_code,multi_method(3),analyte(4)
47     character*30   t_analyte,c_analyte(4)
48     character*2   less_thn,bkgd_subtract,tray_id
49
50     character*3   cup,dum,change_data(40),mode,del
51
52     character*4   serial_number
53
54     character*8   version,blankcor,blanko,low_limit,o_result
```

```

50      character*8    result,a_result,error,u_limit,l_limit
51      character *8   limit,c_low_limit
52      character*10   units(5),a_units,dilute,dollars,seq_number
53      character*11   req_number(40),ident,delete_req(40),msg

54      character*14   prep_proc,anal_proc,filename
55      character*14   t_prep_proc,t_anal_proc
56      character*1     char,ans,c_one,bell
57      character*7    root_sample_id,rep_time,message
58      character*7    c_badge_number
59      character*5    mc
60      character*6    timea,report_date,a_badge_number
61      character*24   weight,badge_number

62      integer*2     i,j,k,l,m,n,i_cup,idum,icount
63      integer*2     in_sample_type,ism,iposition
64      integer*2     lpos,last_req,new_req,itrays
65      integer*2     l_limit_flag,limit_flag,in_count
66      integer*2     k_std,k_blank,k_spec,k_epa,k_pet
67      integer*2     n_outliers,kr_blank,i_analyte(4)
68      integer*2     i_factor,crlf,procedure_flag,del_sample(40)
69      integer*2     delspec(4)
70      real*8       blank(4,40),t_blank(4),r_blank(4)

71      common filler,blanks

72      assign 898 to crlf

73      type *,' Default filename is ''fis.dat'''
74      type *,' Enter new filename,or hit ENTER to use default'
75      accept 252,filename
76      if (filename(1:1) .eq. ' ') go to 119
77      go to 1019

78      1018     type 101,' Enter filename (and extension) to read
79      1 [eg: 123nmf.rpt]: '
80      accept 252,filename
81      101      format (a58,$)
82      go to 1019
83      119      filename = 'fis.dat'
84      1019     open (unit=15,file=filename,err=1018,status='old',
85      1         form='formatted',access='sequential',readonly)

86      open (unit=16,file='tempo1.dat',
87      1         status='new',form='formatted',
88      1         access='sequential')

89      open (unit=18,file='file_transfer.dat',
90      1         status='unknown',form='formatted',
91      1         access='sequential')
92      i_bell = 7
93      write (bell,'(a1)')i_bell
94      dollars = '$$'
95      l_limit = ''
96      dum = ''
97      last_pass = 0
98      blanks=''
99      method =
100     method_code = method
101     t_method_code = method
102     analysis = method
103     a_method_code = method
104     i_badge_number = 0
105     in_sample_type = 1
106     bkgd_subtract = '-B'

```

```

107          icount=0
108          prep_proc = ' '
109          anal_proc = ' '
110          t_prep_proc = ' '
111          t_anal_proc = ' '
112          error = ' '
113          ans = ' '
114          char = ' '
115          c_one = ' '
116          tray_id = ' '
117          ncount = 0
118          in_count = 0
119          lt_count = 0
120          kdel = 0
121          n_outliers = 0
122          version = '9/20/88'

123      ! Get the sample header data

124      5      call read_filler
125      if (filler .eq. blanks) go to 5

126      if (filler(1:12) .eq. ' End of data') goto 700

127      59     if (filler(19:26) .ne. 'QuikCalc') go to 5 ! skip blank lines

128      !start of text found--get date and time of analysis

129      6      call read_filler
130      if (filler .eq. blanks ) go to 6
131      name = 0
132      if (filler(1:12) .eq. ' End of data') then
133          type *, ' Exit at 6' ! This is the normal exit point
134          goto 700
135      end if

136      do i = 1,128
137          req_del(i:i) = ' '
138      end do
139      icount = icount + 1
140      report_date = filler(34:43)
141      rep_time = filler(46:52)
142      timea(1:2) = filler(46:47)
143      timea(3:6) = filler(49:52)
144      report_date(1:2)= filler(42:43)
145      report_date(3:4) = filler(34:35)
146      report_date(5:6) = filler(37:38)
147      tray_id(1:2) = filler(39:40)
148      if (report_date(3:3) .eq. ' ') report_date(3:3) = '0'
149      if (report_date(5:5) .eq. ' ') report_date(5:5) = '0'
150      if (timea(3:3) .eq. ' ') timea(3:3) = '0'
151      if (timea(1:1) .eq. ' ') timea(1:1) = '0'

152      ! Date has the format yymmdd ; time in 2400 format
153      !
154      !      type *,report_date,' ',timea
155      ! Clear req #'s from memory area

156      do i=1,40
157          req_number(i)= ' '
158          delete_req(i) = req_number(i)
159          del_sample(i) = 0
160      end do

161      ! get method code

```

```

162      250    call read_filler
163          if (filler(1:1) .eq.'T') Seq_number = filler (44:52)
164          if (filler(1:1) .ne. 'M' ) go to 250
165          method = filler(9:32)

166          do i=1,30                                ! Left-justify 'method'
167              if (method(1:1) .ne. ' ') go to 10
168              method(1:29) = method(2:30)
169              method(30:30)=' '
170          end do

171      10      continue

172      ! Look for multiple analyses
173      n_slash = 0
174      do ij = 1,3
175          char = ' '
176          do i = 1,30
177              char = filler(i:i)
178              if (char .ne. '/') then
179                  multi_method(ij)(ij:ij) = filler (i-n_slash:i-n_slash)
180              end if
181          end do
182          if (i .lt. 31) n_slash = i
183          if (i .ge. 30 .and. char .ne. '/') go to 11
184      end do
185      do i = 1,3
186          type *,multi_method(i)
187      end do

188      11      do i= 1,20
189          type crlf
190      end do

191      type *,',method,' : analysis performed on FIS','',
192      1 report_date,' ',timea
193      type *,' Sequence # (ref): ',seq_number
194      type crlf

195      if (analysis .ne. method ) then           ! Clear default
196          prep_proc = ' '
197          anal_proc = ' '
198      end if

199      ! Get badge number of operator

200      2120    badge_number = filler(34:56)           ! Includes 'Operator'
201      ipos=index(badge_number,:)
202      c_badge_number = badge_number(ipos+1:ipos+8)
203      if (c_badge_number .eq. ' ' .or. ipos .eq. 1) then
204          type 21, ' Missing or incorrect badge #; please correct:'
205          c_badge_number = ' '
206          accept 252, c_badge_number
207      end if
208      21      format (a46,$)

209      ! justify badge #

210      do i=1,6
211          if (c_badge_number(6:6) .ne. ' ') go to 15
212          c_badge_number(2:6) = c_badge_number(1:5)
213          c_badge_number(1:1) = ' '
214      end do

```

```

215      ! Check for all-numeral badge number

216      15      do i=2,6
217          if (c_badge_number(i:i) .eq. ' ') go to 2120
218          if(c_badge_number(i:i).lt.'0'.or.c_badge_number(i:i).gt.'9')then
219              ipos =1
220              go to 2120
221          end if
222          ipos=0
223      end do

224      ! get request numbers.  Tray Comments .  Each req # is followed by '!'
225      1555    call read_filler
226          if (filler .eq. blanks ) goto 1555
227          155    if (filler(1:14) .eq. 'Tray Comments:') then !line 6
228              j = 0
229              i_cup = j
230              i_position = 15

231      16      do j = 1,40      ! req_number length is 11 chars
232          req_number(j) = ' '
233          k=1
234          171    continue
235          17      do i = i_position+1,60
236              char = ' '
237              char = filler(i:i)
238              if (char.ne. ';' .and.(char.lt.'0'.or.char.gt.'9'))then
239                  call read_filler
240                  if (filler .eq. blanks) go to 118
241                  i_position =15
242                  go to 171
243              end if
244              i_position = i
245              req_number(j)(k:k) = char
246              k=k+1
247              if (char .eq. ';') go to 18   ! end of one request #
248              if (i .ge. 60 ) then
249                  118      call read_filler
250                  if (filler .eq. blanks) goto 118 !line 7 or 8
251                  i_position = 0
252                  if (filler(6:9) .eq. 'Anal') go to 1150 !line 9
253                  go to 171
254              end if
255          end do
256          18      continue
257      end do
258      if (j-1 .eq. 0) go to 1190
259      1150    continue
260      kl_pos = 4
261      if (filler(17:24) .eq. '        ')then !line 9 (Analyte ->)
262          type *, ' No analysis name--cannot process'
263          type *, bell
264          go to 59
265      end if
266      if (filler(17:17) .eq. ' ')then
267          filler(17:23) = filler(18:24)
268          filler(24:24) = ' '
269          go to 1150
270      end if
271      analyte(1) = filler(17:45)
272      analyte(2) = filler(17:23)
273      analyte(3) = filler(28:34)
274      analyte(4) = filler(39:45)
275      if (analyte(4) .eq. '        ') then

```

```

276      if(analyte(3) .eq. ' ') analyte(2) = analyte(1)
277      end if
278      if (analyte(3) .eq. ' ') kl_pos = kl_pos - 1
279      if (analyte(2) .eq. ' ') kl_pos = kl_pos - 1
280 !     type *, ' kl_pos = ',kl_pos

281      1190 type *,' Request Numbers:'
282      newreq = 0
283      do i = 1,j-1
284          ipos = index(req_number(i),';')
285          req_number(i)(4:4+ipos-1)=req_number(i)(1:ipos)
286          req_number(i)(1:3) = 'EAL'
287          do k= 1,10
288              if (req_number(i)(4:4) .eq. ' ') then
289                  req_number(i)(4:10) = req_number(i)(5:11)
290                  req_number(i)(11:11) = ' '
291              end if
292          end do ! <k>
293          ipos = index(req_number(i),';')
294          if (ipos .ne. 0 ) req_number(i)(ipos:ipos) = ' '
295          ic_flag=0
296      end do ! <i>
297      n_requests = j-1
298      j= 1
299      do i = 1,(n_requests/4)+1
300          type 181,' ',req_number(j),' ',req_number(j+1),
301          1      ' ',req_number(j+2),' ',req_number(j+3)
302          j= j+4
303          if (j.ge.n_requests)go to 1181
304      end do
305      1181 type *,' Total requests = ',n_requests

306      181 format ( 4(a3,a11,$))
307      end if

308      ! find units of measurement

309      1200 call read_filler
310      if (filler .eq. blanks ) goto 1200
311      if (filler(19:23) .eq. 'QuikC') goto 6
312      if (filler(1:3) .ne. 'Cup' ) go to 1200

313      units(2) = ' '
314      units(2) = filler(18:23)
315      units(3) = ' '
316      units(3) = filler (29:34)
317      units(4) = ' '
318      units(4) = filler (40:45)
319      units(5) = ' '
320      units(5) = filler (51:56)
321      do i = 1,4
322          lpos=10
323          do while (lpos .gt. 1)
324              lpos=index(units(i), ' ')
325              if (lpos .eq.0) goto 1260
326              units(i)(1:9) = units(i)(2:10)
327          end do
328      end do

329      !     in_sample_type 1 = sample
330      !             2 = water blank
331      !             3 = standard
332      !             4 = reagent blank
333      !             5 = EPA standard

```

```

334      !           6 = Pet sample
335      !           7 = Something else
336      !           8 = Deleted sample
337      !           these definitions can be expanded for other categories

338      ! Read the sample data area and store results on disc

339          if (filler(1:12) .eq. ' End of data') then
340              type *, ' End at 1260'
341              goto 700
342          end if

343      1260    continue
344          i_blank_found = 0
345          last_req = 0
346          root_sample_id = ''
347          serial_number = ''
348          ident = ''
349          sample_number = ''
350          npos = 40

351          do i=1,4
352              do j=1,40
353                  blank(i,j) = 0.0
354              end do
355              r_blank(i) = 0.0
356              t_blank(i) = 0.0
357          end do

358      39      type *, ' New tray-- hit ENTER to continue, or ''$'' to skip tray'
359          type *, bell
360          accept 252,ans
361          if (ans .eq.'$') go to 59
362          if (ans .ne. ' ') go to 39

363          ! Select species to report
364          isum = 0
365          i_analyte(1) = 0
366          do i = 2,4
367              if (analyte(i) .ne. '') isum = isum + 1
368              i_analyte(i) = 1
369          end do
370          ! type *, ' isum ',isum
371          if (isum .gt. 1) then
372              type *, bell
373              type *, ' Select analytes to report:'
374              do i = 2,isum+1
375                  type *, ' ',i-1,' - ',analyte(i)(1:10)
376                  i_analyte(i) = 0
377              end do
378          ans = ' '
379          type *, ' Hit ENTER to report all analytes, or '
380          type *, ' enter the NUMBER(s) of the analyte(s) you want to report.'
381          accept 252,ans
382          if (ans.eq.' ') then
383              do i = 2,4
384                  i_analyte(i) = 1
385              end do
386              go to 177
387          end if
388          do i = 2,isum+1
389              if (ans .eq. ' ') go to 177
390              if (ans .lt. '0' .or. ans.gt.'9') go to 175
391              read (ans,'(f2.0)')r_ans
392              if (r_ans.lt.0 .or. r_ans .gt. isum) go to 175

```

```

393      i_analyte(r_ans + 1) = 1
394      ans = ''
395      if (i .lt.i.sum+1)then
396          type *,' Enter next number;terminate list with ENTER only'
397          accept 252,ans
398      end if
399      end do
400      end if
401
402 ! Select whether to enter request #'s to use or those to delete
403 177  if (n_requests.gt.1) then
404      nx = 0
405 179  continue
406      type crlf
407      type *,' Enter ''$'' if you want to process data by request # '
408      type *,' Hit ENTER to process all requests'
409      type *, bell
410      accept 252,ans
411      if (ans.ne.'$'.and.ans.ne.' ') go to 179
412      if (ans.eq.'$') then
413          ans= ''
414          type *,' OPTION: S(ave) or D(elete) ?'
415          type crlf
416          type *,' If you (S)ave one or more requests, only those ''saved'''
417          type *,' will be processed.'
418
419          type *,' If you (D)elete one or more requests, those not deleted'
420          type *,' will be processed.'
421          type crlf
422          type *,' Valid requests : '
423          j = 1
424          do i = 1,(n_requests/4)+1
425              type 181,' ',req_number(j),' ',req_number(j+1),
426              ' ',req_number(j+2),' ',req_number(j+3)
427              j= j+4
428              if (j.ge.n_requests)go to 1791
429          end do
430          nx = 0
431          type *,' Please enter S or D'
432          accept 252, ans
433          do i = 1,128
434              req_del(i:i) = ''
435          end do
436          do i = 1,40
437              delete_req(i) = ''
438          end do
439          nq = 1
440          if (ans.eq.'S'.or.ans.eq.'s')then
441              nq = 0
442              msg='to save: '
443              go to 1792
444          end if
445          if (ans.eq.'D'.or.ans.eq.'d')then
446              nq = 0
447              msg = 'to delete: '
448              go to 1792
449          end if
450          if (nq) then
451              msg = '           ! 11 spaces
452              ans = ''
453              go to 1791
454          end if
455 1792  type *,' Enter the request #(s) ',msg
        type *,' EXAMPLE: 9996;9975;...;9966(no spaces,do not enter EAL)'

```

```

456      type *, ' Hit ENTER to process all requests.'
457      accept 252,req_del
458      if (req_del(1:1).eq.' ') go to 1239
459      do j = 1,11 * n_requests
460      if (req_del(j:j) .eq. ';' .or. req_del(j:j).eq.' ') go to 1241
461          if (req_del(j:j).lt.'0' .or. req_del(j:j).gt.'9')then
462              type *, ' Entry ERROR; please re-enter request #'
463              do jk = 1,128
464                  req_del = ' '
465              end do
466              type crlf
467              type *, ' Valid requests : '
468              do jk= 1,n_requests
469                  type *, ' ',req_number(jk)
470              end do
471              go to 1792
472          end if
473      1241      continue
474      end do
475      ndel = 0
476      n = 1
477      m = 11
478      do j = 1,n_requests
479          i = n
480          nc=1
481          do ii = i,m+i-1
482              char = req_del(ii:ii)
483              if (char.eq.' ' .and. nc.eq.1) goto 1820
484              if (char.eq.' ' .and. ii.eq.10+i) go to 1820
485              if (char .eq. ';' .or. char.eq. ' ') then
486                  ndel = ndel +1
487                  n = ii+1
488                  go to 1810
489              end if
490              if (req_del(ii:ii).ge.'0' .and. req_del(ii:ii).le.'9') then
491                  delete_req(j)(nc:nc) = req_del(ii:ii)
492                  nc = nc + 1
493              end if
494              end do
495      1810      continue
496      end do
497      1820      type crlf
498      type *, ' Number of requests ',msg,'= ',ndel
499      if (ndel.gt.n_requests)then
500          type *, ' There are only ',n_requests,' request #'s'
501          go to 179
502      end if

503      type crlf
504      do i = 1,ndel
505          do j= 1,11
506              if (delete_req(i)(1:1) .eq. ' ')then ! Left justify
507                  delete_req(i)(1:10) = delete_req(i)(2:11)
508                  delete_req(i)(11:11) = ' '
509              end if
510          end do
511          delete_req(i)(4:11) = delete_req(i)(1:8)
512          delete_req(i)(1:3) = 'EAL'
513      end do
514      do nx = 1,n_requests
515          ns = 0
516          do nk = 1,n_requests
517              if (delete_req(nk)(4:11) .ne. ' ')then
518                  if (delete_req(nx).eq.delete_req(nk))then
519                      ns=ns+1

```



```

583         if (l_limit(i:i).lt.'0'.or.l_limit(i:i).gt.'9')go to 45
584         end if
585         end do
586         do i = ipos+1,8
587             if (l_limit(i:i).lt.'0'.or.l_limit(i:i).gt.'9')goto 45
588             end do
589         end if
590         l_limit_flag = 1
591         i_blanksub = 0
592         do j = 1,npos      ! there are 40 positions on sample trays      *
593     !
594     ! ****
595         if (kl .eq. 1) then ! One time thru to find blanks
596         126     call read_filler
597             if (filler .eq. blanks ) go to 126
598             if (filler(1:12) .eq. ' End of data') goto 2521
599             if (filler(19:26).ne.'QuikCalc')type *,,' Cup # ',filler
600             if (filler(19:26) .eq. 'QuikCalc' )then
601             2521     if (i_blank_found .gt. 1)then
602                 type crlf
603                 type *,,' There is more than one reagent blank. '
604                 type *,,bell
605                 do i = 2,kl_pos-1
606                     if(i_analyte(i) .ne. 1) go to 200
607                     type crlf
608             2522     type *,,' To select blank result to use, '
609                 type *,,'    enter A, M(ean), N(new) or D(delete).'
610                 type crlf
611                 type *,,' A- Values for ',analyte(i),': '
612                 do ii= 1,i_blank_found
613                     type 254, ii,blank(i,ii)
614                 end do
615                 type 255,' Mean blank is      : ',t_blank(i)
616                 ans = ''
617                 l_point = 0
618                 accept 252,ans
619                 if (ans .eq. 'A'.or.ans.eq.'a') then
620                     message = 'use: '
621                     l_point = 1
622                 end if
623                 if (ans .eq. 'D'.or.ans.eq.'d') then
624                     message = 'delete:'
625                     l_point = 2
626                 end if
627                 if (l_point .lt.1) go to 2526
628             2523     type *,,' Please enter the NUMBER of the blank to ',message
629                 accept 252,dum
630                 do ii = 1,3
631                     if (dum(3:3) .eq.' ')then
632                         dum(2:3) = dum(1:2)
633                         dum(1:1) = '0'
634                     end if
635                 end do
636                 do ii=1,3
637                     if (dum(ii:ii).lt.'0'.or.dum(ii:ii).gt.'9') go to 2523
638                     end do
639                     read(dum,'(i3)')num
640
641                     if (l_point .eq. 1 )r_blank(i) = blank(i,num)
642                     if (l_point .eq. 2 )then
643                         r_blank(i) = 0.0
644                         blank(i,num) = 0.0
645                         sum = 0.0
646                         do ii = 1,i_blank_found
647                             sum = sum + blank(i,ii)

```

```

647           end do
648           i_blank = i_blank_found-1
649           if (i_blank.gt.0) t_blank(i) = sum/(i_blank)
650           go to 2522
651           end if
652
653           2526   if (ans .eq. 'M'.or.ans.eq.'m')then
654               r_blank(i)=t_blank(i)
655               l_point = 3
656           end if
657           if (ans .eq. 'N'.or.ans.eq.'n')then
658               type 253,' Enter blank value: '
659               l_point = 4
660               accept 252,blankcor
661               do ii = 1,8
662                   if (blankcor(8:8) .eq. ' ') then
663                       blankcor(2:8) = blankcor(1:7)
664                       blankcor(1:1) = ' '
665                   end if
666               end do
667
668           !           read (blankcor,'(f8.3)')blank(i,i_blank_found)
669           !
670           !           type *,',',analyte(),' blank: ',blankcor
671           !           type *,',',r_blank(i)
672           !           r_blank(i)= blank(i,i_blank_found)
673           end if
674           if (l_point .lt. 1)then ! No selection made,repeat.
675               type *,bell
676               go to 2522
677           end if
678           ans = ' '
679
680           200  continue
681           end do
682           end if
683           npos = j -1
684           fill_buf(42)=filler
685           go to 9100
686           end if
687           do i = 1,3
688               char = filler(i:i)
689               if (char.ne.' ') then
690                   if (char.lt.'0'.or.char.gt.'9')go to 99
691               end if
692           end do
693           read (filler(1:3),'(i3)')i_fill
694           npos = i_fill
695           fill_buf(i_fill) = filler      !store a line of data
696
697           ! If there are reagent blanks, get blank data
698
699           if (filler(5:5) .eq. 'b' .or. filler(5:5).eq.'B')then
700               i_blank_found = i_blank_found + 1
701               type *,',',i_blank_found '=',i_blank_found
702               do i=1,kl_pos-2
703                   blanko=filler(16+(i-1)*11:23+(i-1)*11)
704                   do ii = 1,8
705                       if (blanko(ii:ii) .eq. '<') blanko = '0000.000'
706                   end do
707                   blankcor = blanko
708                   do ii = 1,8
709                       if (blankcor(8:8) .eq. ' ') then
710                           blankcor(2:8) = blankcor(1:7)
711                           blankcor(1:1) = ' '
712                   end if

```

```

708      end do

709      read (blankcor,'(f8.3)')blank(i+1,i_blank_found)
710      r_blank(i+1) = blank(i+1,i_blank_found)
711      sum = 0.0
712      do ii = 1,i_blank_found
713          sum = sum + blank(i+1,ii)
714      end do

715      t_blank(i+1) = sum/i_blank_found

716      type *, ' ',analyte(i+1),' blank: ',blankcor

717      ! Blank(n,m) is the REAL value of the reagent blank.
718      ! Blankcor is the STRING representation of the blank as read from filter.
719      ! t_blank is the REAL mean when more than one reagent blank is found

720      253      format(a20,$)
721      254      format(i3,f6.3)
722      255      format(a24,f6.3)
723      2555     blankcor = '0000.000'
724      end do  !'blank' is reagent blank
725      end if
726      ! filler (1:12) = '
727      go to 9099
728      end if

729      ! End of first pass from line 126
730      40      continue

731      !
732      ! *****
733      ! * Find Sample Type *
734      ! *****
735      !      type *, ' ***** Pass # ',kl,' line # ',j
736      !      filler = fill_buf(j)
737      !      cup = fill_buf(j)(1:3)
738      !      do ik = 1,3
739          !      if(cup(3:3).eq.' ')then
740          !          cup(2:3)= cup(1:2)
741          !          cup(1:1) = '0'
742          !      end if
743      end do
744      read(cup,'(i3)')i_cup
745      if (i_analyte(kl) .ne. 1) go to 99
746      method(1:3) = analyte(kl)(1:3)
747      a_units = units(kl)

748      41      in_sample_type = 1
749      char = filler(5:5)
750      if (char .gt. '9' ) then
751          if (char .eq. 'S' .or. char .eq. 's') then
752              if (filler(6:6) .eq.'E'.or.filler(6:6).eq.'e')goto 411
753              in_sample_type = 3
754              if (kl .le.2)k_std = k_std + 1
755              type *, ' :standard & result : ',filler(6:11),',',
756              1 filler(16+(kl-2)*11:23+(kl-2)*11)
757              else if (char .eq. 'H'.or.char.eq.'h' ) then
758                  if (kl .le.2)k_blank = k_blank + 1
759                  in_sample_type = 2
760                  type *, ' :water blank & result : ',
761                  1 filler(16+(kl-2)*11:23+(kl-2)*11)
762                  else if (char .eq. 'b' .or. char .eq. 'B') then
763                      if (kl .le. 2)kr_blank = kr_blank + 1

```

```

763          in_sample_type = 4
764          type *, ' :reagent blank & result : ',
765          1 filler(16+(kl-2)*11:23+(kl-2)*11)
766          else if (char .eq. 'E'.or.char.eq.'e' ) then
767          411      in_sample_type = 5
768          if (kl .le. 2)k_epa = k_epa + 1
769          type *, ' EPA standard'
770          else if (char .eq. 'P'.or.char.eq.'p' ) then
771          in_sample_type = 6
772          if (kl .le.2)k_pet = k_pet + 1
773          type *, ' Pet sample'
774          else
775          in_sample_type = 7
776          if (kl .le. 2)k_spec = k_spec + 1
777          type *, ' special material & results :',filler(5:46)
778          end if

779          if (in_sample_type .ne. 1) then
780          serial_number = ' '
781          ident = ' '
782          sample_number = ' '
783          end if
784          end if

785          !      type *, ' in_sample_type = : ',in_sample_type
786          251      format (a39,$)
787          252      format (a)

788          !227
789          !  real samples
790          !  There may be spiked samples and/or duplicates.
791          !  Duplicates will be reported, spiked samples will not.

792          !      type *, ' You have arrived at sample data area '
793          !      type *, ' in_sample_type = ',in_sample_type

794          if ( in_sample_type .ne.1 ) go to 99

795          ! Detect end of tray

796          if (filler(1:3) .eq. ' ' ) goto 59
797          do i = 1,3      ! skip garbled entries
798          char = filler(i:i)
799          if (char.ne.' ')then
800          if(char.lt.'0'.or.char.gt.'9')go to 99
801          end if
802          end do
803          ****
804          ! Process sample number area
805          !
806          ident = ' '
807          33      ident = filler(5:15) ! 11 characters in report field
808          ! Several possibilities exist for sample # area:

809          ! Possibility #1 --- New Sample/Req #
810          1170      if (ident(7:7) .eq.'-' ) then ! new sample
811          do i = 1,6                  ! Only numbers allowed
812          if (ident(i:i) .lt. '0' .or. ident .gt. '9') goto 1117
813          end do
814          go to 1171
815          1117      type *, ' Present sample : '

```

```

816      type *,,' ,filler(5:59)
817      type *,,' Enter correct sample # or'
818      type *,,' ''s'' to skip result, or ''d'' to delete sample'
819      accept 252,ident
820      do ii = 1,10
821          if (ident(ii:ii) .eq.'d'.or.ident(ii:ii).eq.'D')then
822              fill_buf(j)(5:5) = 'x'
823              kdel = kdel +(kl_pos-2)
824              go to 9099
825          end if
826          if (ident(ii:ii).eq.'s'.or.ident(ii:ii).eq.'S')then
827              kdel = kdel + 1
828              go to 9099
829          end if
830      end do
831      go to 1170
832      1171      new_req = 1
833          last_req = last_req + 1      ! Match with request #
834          root_sample_id = filler (5:11)
835          ! root_sample id is 'yymmdd-'
836          ident (8:11) = filler (12:15)! Last char may be '+' or 'd',
837          go to 210                  ! so read one additional char.
838      end if                      ! Serial_number = ident(8:10)
839          ! when correctly assembled.
840
! Possibility 2 --- Continuation of previous sample
841
842      ident(8:11) = filler (5:8)
843      if (del_sample(j)) go to 9099
844
! Now check sub_sample # (serial number)
845
846      ! Final serial_number is 3 numerical chars--supply leading zero's.
847      ! There may be 4 char's in the serial number as read.
848      ! At present, duplicates are flagged with a trailing 'd'.
849      ! The following procedure will trap 1,2,or 3-numerical digits
850      ! followed by a 'd'.
851
852      210      char = ident (8:8)
853      2100     continue
854      do i=1,4
855          char = ident(8:8)
856          if (char .eq. ' ') then
857              ident (8:10) = ident (9:11)
858              ident (11:11) = ' '
859          end if
860      end do
861      do i = 1,4
862          if (ident(11:11) .eq. ' ') then
863              do ij=1,3
864                  char = ident(10:10)
865                  if(char.ge.'0'.and.char.le.'9')go to 1111
866                  ident(9:10) = ident(8:9)
867                  ident(8:8) = '0'
868              end do
869          end if
870      end do
871      if (ident(11:11).eq.'d'.or.ident(11:11).eq.'D')go to 1111
872      do i = 8,10
873          ncount = 0
874          if(ident(i:i).lt.'0'.or.ident(i:i).gt.'9')then
875              type *,,' Sub-sample # in error;now,',ident
876              type *,,'bell
877              type *,,' Enter correct sub_sample # or'
878              type *,,' ''s'' to skip result or ''d'' to delete sample: '
879              accept 252,ident(8:10)
880              do ii = 8,11

```

```

878      if (ident(ii:ii) .eq. 'd'.or. ident(ii:ii).eq.'D') then
879          fill_buf(j)(5:5) = 'x'
880          kdel = kdel +kl_pos-2
881          go to 9099
882      end if
883      if (ident(ii:ii).eq.'s'.or.ident(ii:ii).eq.'S')then
884          kdel=kdel +1
885          go to 9099
886      end if
887  end do
888  end if
889  end do
890  1111    serial_number (1:3) = ident (8:10)

891 ! Now assemble the full sample number .
892 ! Final sample_number must have ten chars 'yymmdd-sss', where 'sss'
893 !   stands for 'subsample number'(serial_number).

894  1110    sample_number (1:7) = root_sample_id
895    sample_number (8:10) = serial_number
896    c_sample_number = sample_number

897  do i = 1,10
898      if (sample_number(i:i) .eq. ' ') go to 1171
899  end do

900  if (new_req .eq.1) fill_buf(j)(5:14) = sample_number
901  if (ident(1:3) .ne. root_sample_id(1:3))then
902      fill_buf(j)(5:8)=serial_number
903      fill_buf(j)(9:15) = ' '
904  end if

905 ! Possibility #3 --- Spiked, or sample too small; do not include in report

906  do i=5,15
907      if (filler(i:i) .eq. '+') then  !spiked
908          filler(5:5) = 'x'
909          go to 99
910      end if
911      if (filler(i:i) .eq.'Q'.or.filler(i:i).eq.'q')then
912          filler(5:5) = 'x'
913          go to 99
914      end if
915  end do
916  1055    if (new_req .eq. 1 ) then

917 ! Now edit in customer-specific requirements
918 ! List request number and match with conversions to be performed

919      char = ' '
920      if (last_req .gt. n_requests) last_req = 1
921      ind = last_req
922      change_data(ind) = ' '
923      if (nx) then
924          do i = 1,n_requests
925              if (req_number(ind).eq.delete_req(i))go to 160
926          end do
927          go to 99
928      end if
929      if (nx.eq. 0)then
930          do i = 1,n_requests
931              if (req_number(ind).eq.delete_req(i))go to 99
932          end do
933      end if
934      continue
160

```

```

935      type crlf
936      type *, ' SELECT OPTIONS -- Request # : ',req_number(ind)
937      ic_flag= 0
938      c_one = ' '
939      c_low_limit = ' '
940      type*, ' Enter customer value for detection limit;otherwise,ENTER.'
941      accept 252, c_low_limit
942      do i = 1,8
943      char = c_low_limit(i:i)
944      if (char.ne.' ')then
945      if (char.ne.'.' and char.lt.'0' or char.gt.'9') go to 160
946      end if
947      end do
948      1156      read (c_low_limit,'(f8.5)')customer_limit
949      read(l_limit,'(f8.5)')xl_limit
950      if (customer_limit .lt. xl_limit)then
951          c_low_limit = l_limit
952          go to 1156
953      end if
954      !
955      ! Eliminate unwanted results
956      !
957      ans = ' '
958      i_del = 0
959      do ix = 1,40
960      del_sample(ix) = 0
961      end do
962      1158      type *, ' Do you want to eliminate any results?<y=yes,ENTER=no>'
963      accept 252,ans
964      if (ans .eq. ' ') go to 1160
965      if (ans .ne.'y'.and.ans.ne.'Y')go to 1158
966      type *, ' Enter the cup numbers of the samples to delete;'
967      type *, ' end input with blank(ENTER).'
968      n_cup = i_cup
969      do ij = i_cup,npos
970      1258      del = ' '
971      i_del =0
972      type *, ' Enter Cup # to delete:'
973      accept 252, del
974      if (del(1:1).eq.' ') go to 1460
975      do ix = 1,3
976          if (del(3:3).eq.' ')then
977              del(2:3) = del(1:2)
978              del(1:1) = '0'
979          end if
980      end do
981      read(del,'(i3)')i_del
982      type *, i_del
983      if(i_del.gt.0)then
984          if (i_del.lt.n_cup)then
985              type *, ' Your request cannot be honored for cup',i_cup
986              type *, ' Data for this sample already processed'
987              type *, ' Hit ENTER to continue'
988              accept 252, ans
989              go to 1258
990          end if
991          if (i_del .gt. npos)then
992              type *, ' No such sample; try again'
993              go to 1258
994          end if
995          del_sample(i_del) = 1
996          type *, ' del ',del_sample(i_del)
997      end if
998      1459      end do

```

```

999      1460  type *,,' Samples to be deleted for this analyte:'
1000          type *,,' Cup To delete'
1001          delspec(kl)=0
1002          do ix = 1,npos
1003              if(del_sample(ix)) then
1004                  type 1461,' ',ix,' ', fill_buf(ix)(5:59)
1005                  delspec(kl)=delspec(kl)+1
1006              end if
1007          end do
1008          1461  format (a4,i3,a3,a55)
1009          1350  type *,,' Are there any changes?<y=yes;ENTER = no>'
1010          ans= ' '
1011          accept 252,ans
1012          if(ans.eq.' ')go to 1160
1013          if (ans.ne.'y'.and.ans.ne.'Y')go to 1350
1014          do ix = 1,40
1015              del_sample(ix) = 0
1016          end do
1017          type *,,' Previous selections deleted'
1018          go to 1158
1019          1160  nit = 0
1020          ans = ' '
1021          if(method(1:3) .eq.'NO3') nit = 1
1022          if(method(1:3) .eq.'TKN') nit = 1
1023          if(method(1:2) .eq.'TN' ) nit = 1
1024          if (nit) then
1025              kickback = -1
1026              ipos = index (req_number(ind),';')
1027              t_method_code = 'N
1028              type 555,' Enter ''N'' to convert to ''NO3'' : '
1029              accept 252,c_one
1030              if (c_one.eq.'N'.or.c_one.eq.'n')then
1031                  t_method_code = 'NO3 '
1032                  ic_flag = 1
1033                  go to 161
1034              end if
1035              if (c_one .ne. ' ') go to 160      ! Error in entry
1036          161   mc(1:5) = t_method_code(1:5)
1037          type *,,' Report nitrate as [',mc,' = default] : '
1038          accept 252,a_method_code
1039          ans = ' '
1040          1610  type 1010, ' Change Procedure #'s ? <y = yes;ENTER = no>
1041          accept 252, ans
1042          if ( ans .eq. 'y' .or. ans .eq. 'Y' )then
1043              procedure_flag = 1
1044              prep_proc = 'To be changed '
1045              anal_proc = 'To be changed '
1046              go to 1612
1047          end if
1048          if (ans.ne.' ')then
1049              type *,,bell
1050              go to 1610
1051          end if
1052          1612  method_code = a_method_code
1053          if (a_method_code(1:1) .eq. ' ') then
1054              method_code = t_method_code
1055              goto 121
1056          end if
1057      end if
1058      1010  format (a44,$)
1059      111   iphos = 0
1060          if (method(1:3).eq.'PO4')iphos = 1
1061          if (method(1:3).eq.'TKP')iphos = 1
1062          if (method(1:2).eq.'TP') iphos = 1
1063          if (iphos) then

```

```

1064         kickback = 0
1065         t_method_code = 'P'
1066         method_code = t_method_code
1067         c_one = ' '
1068         ic_flag= 0
1069         type 555,' Enter ''P'' to convert to another species :'
1070         accept 252, c_one
1071         if (c_one .eq.'p'.or.c_one .eq.'P') then
1072             ans = ' '
1073             type *, ' Enter the NUMBER of the conversion to make:'
1074             type crlf
1075             type *, ' 0--> P (no change)'
1076             type *, ' 1--> PO4'
1077             type *, ' 2--> H3PO4'
1078             type *, ' 3--> P2O3'
1079             type *, ' 4--> P2O4'
1080             type *, ' 5--> P2O5'
1081             accept 252,ans
1082             if (ans .eq. ' ')then
1083                 type *,bell
1084                 go to 111
1085             end if
1086             if (ans .lt. '0' .or. ans .gt. '5')then
1087                 type *,bell
1088                 go to 111
1089             end if
1090             t_method_code = 'P'
1091             if (ans .eq. '0' )then
1092                 t_method_code(1:5) ='P'
1093                 factor = 1.0
1094             end if
1095             if (ans .eq. '1' )then
1096                 t_method_code(1:5) = 'PO4'
1097                 factor = 3.0661
1098             end if
1099             if (ans .eq. '2' )then
1100                 t_method_code(1:5) = 'H3PO4'
1101                 factor = 98.0/30.9738
1102             end if
1103             if (ans .eq. '3' ) then
1104                 factor = 109.95/(30.9738*2)
1105                 t_method_code(1:5) = 'P2O3'
1106             end if
1107             if (ans .eq. '4' ) then
1108                 factor = 125.95/(30.9738*2)
1109                 t_method_code(1:5) = 'P2O4'
1110             end if
1111             if (ans .eq. '5' ) then
1112                 factor = 2.29136
1113                 t_method_code(1:5) = 'P2O5'
1114             end if
1115             if (ans .ne. '0') ic_flag = 1
1116         end if
1117         type *, ' Report phosphate as [',t_method_code(1:5),', = default] :'
1118         accept 252,a_method_code
1119         400 type 1010, ' Change Procedure #' ? <y = yes;ENTER = no>
1120         accept 252, ans
1121         if ( ans .eq. 'y' .or. ans .eq. 'Y' )then
1122             procedure_flag = 1
1123             prep_proc = 'To be changed'
1124             anal_proc = 'To be changed'
1125             go to 410
1126         end if
1127         if (ans .ne. ' ')then
1128             type *,bell

```

```

1129          go to 400
1130      end if
1131 410      method_code = a_method_code
1132      if (a_method_code(1:1) .eq. ' ')method_code = t_method_code
1133  end if

1134 4555      if (method(1:3) .eq. 'NH3') then
1135          kickback = 1
1136          t_method_code = 'N'
1137          c_one = ' '
1138          ic_flag= 0
1139          type 556,' Enter ''3'' to convert ''N'' to ''NH3'' : '
1140          type 556,' Enter ''4'' to convert ''N'' to ''NH4'' : '
1141          accept 252, c_one
1142          if (c_one .eq.'3') t_method_code = 'NH3'
1143          if (c_one .eq.'4') t_method_code = 'NH4'
1144          if (c_one .eq.'3'.or.c_one.eq.'4')ic_flag=1
1145  if(c_one.ne.'3'.and.c_one.ne.'4'.and.c_one.ne.' ') go to 4555

1146          type *,' Report ammonia as [',t_method_code(1:3),', = default] :'
1147          accept 252, a_method_code
1148 1251      type 1010, ' Change Procedure #'? <y = yes;ENTER = no>
1149          accept 252, ans
1150          if ( ans .eq. 'y' .or. ans .eq. 'Y' )then
1151              procedure_flag = 1
1152              prep_proc = 'To be changed '
1153              anal_proc = 'To be changed '
1154              go to 125
1155          end if
1156          if (ans.ne.' ')then
1157              type *,bell
1158              go to 1251
1159          end if
1160 125       method_code = t_method_code
1161          if (a_method_code(1:1) .ne. ' ')method_code =a_method_code
1162  end if
1163 555       format (a42,$)
1164 556       format (a37,$)

1165 121       type crlf
1166          do i = 1,30
1167              if (method_code(1:1) .ne. ' ') go to 1211
1168              method_code(1:29) = method_code(2:30)
1169              method_code(30:30) = ' '
1170          end do
1171  !        if (last_req .gt. n_requests) last_req = 1
1172 1211      change_data(last_req)(1:1) = c_one
1173      type crlf
1174          type *, ' Request #:',req_number(last_req)
1175          i_blanksub = 0
1176          type *, ' You have selected the following options: '
1177          if (c_one .eq. 'p' .or. c_one .eq. 'P')type *,
1178              1'           Convert P to : ',t_method_code
1179          if (c_one .eq. 'n' .or. c_one .eq. 'N') type *,
1180              1'           Convert N to NO3'
1181          if (c_one .eq. '3') type *,'           Convert N to NH3'
1182          if (c_one .eq.'4') type *,'           Convert N to NH4'
1183          if (c_one .eq.' ' .and. method(1:3) .eq. 'NO3') type *,
1184              1'           N to be reported as N'
1185          if (c_one .eq. ' ' .and. method(1:3) .eq. 'NH3') type *,
1186              1'           NH3 to be reported as N'
1187          if (c_one .eq. ' ' .and. method(1:1) .eq. 'P') type *,
1188              1'           P to be reported as P'
1189          type *,'           Analysis Name : ',method_code
1190          type *,'           Preparation Procedure # : ',prep_proc

```

```

1191      type *,' Analytical Procedure # : ',anal_proc
1192      if (r_blank(kl) .ne. 0.0) then
1193          if (i_blanksub .eq. 1) go to 1216
1194          type *,' Enter ''c'' to subtract reagent blank;'
1195          type *,' ENTER = no blank correction'
1196          accept 252,ans
1197          if (ans .ne.' ') i_blanksub = 1
1198          ans = ' '
1199          end if
1200      1223      type 1224,' Hit ENTER if OK; any number or letter to change : '
1201          accept 252, ans
1202          if (ans .ne. ' ') goto 160
1203          ans = ' '
1204      1224      format (a51,$)
1205          end if
1206      ! Interpret out-of-limits designations and insert in 2-char field;
1207      ! second char is 'blank'.
1208      1216      char = ' '
1209          char = filler(17+(kl-2)*11:17+(kl-2)*11)
1210          result = ' '
1211          less_thn = ' '
1212          if (char .eq. '<') then
1213              less_thn = '< '
1214              if(in_sample_type .eq.1)lt_count = lt_count + 1
1215              if (l_limit_flag .eq. 1 )goto 1520
1216      1502      type 251, ' Please enter detection limit for method:'
1217          accept 252, l_limit
1218          type *, ' Is limit = ',l_limit,' ? Type c to change;else ENTER'
1219          accept 252, ans
1220          if (ans .eq. 'c')go to 1502
1221      1520      result = l_limit
1222          l_limit_flag = 1
1223          ans = ' '
1224          go to 1060
1225          end if
1226
1227          do i= 16+(kl-2)*11,20+(kl-2)*11
1228              char = filler(i:i)
1229              if(char.eq.'g'.or.char.eq.'h'.or.char.eq.'i')less_thn='> '
1230              if(char.eq.'G'.or.char.eq.'H'.or.char.eq.'I')less_thn='> '
1231              if (char .eq. '>') less_thn = '> '
1232          end do
1233          if (less_thn .eq. '> ' .and. in_sample_type .eq. 1) then
1234              type *,bell
1235              type *,',sample_number,fill_buf(j)
1236              type *,' High result--no entry in Analis. Hit enter to continue'
1237              accept 252,ans
1238              kdel = kdel +1
1239              n_outliers = n_outliers +1
1240              go to 1060
1241          end if
1242
1243          ! Analytical result
1244
1245      1060      less_thn=' '
1246          result = ' '
1247          result(2:8) = filler(16+(kl-2)*11:23+(kl-2)*11)
1248          continue
1249
1250          if (less_thn .eq. ' ')then
1251              result = filler(16+(kl-2)*11:23+(kl-2)*11)
1252          end if
1253
1254          do i=1,8

```

```

1250      if (result(8:8) .eq. ' ') result(2:8) = result(1:7)
1251      result(1:1)=' '
1252  end do
1253  o_result = result ! Save original result
1254  if ( in_sample_type .eq. 4) blankcor = result
1255 ! ****
1256 1061  a_result = result      ! a_result is the reported variable
1257 1062  continue
1258 ! all data in--header and results for one measurement !
1259  if (del_sample(j)) go to 650
1260  if (procedure_flag)then
1261      prep_proc = ' '
1262      anal_proc = ' '
1263  end if
1264  if ( analysis .eq. method .and. procedure_flag .eq.0) go to 650
1265 1100  if (in_sample_type .eq. 1) then
1266      do i=1,14
1267          if (prep_proc(i:i) .ne. ' ') go to 600
1268      end do
1269 ! If preparation or analytical procedures are to be changed, enter here
1270 580      if (i .ge. 14 ) then
1271          prep_proc = ' '
1272          if (procedure_flag)then
1273              type *,bell
1274              type 591,' Enter preparation procedure # : '
1275              go to 592
1276          end if
1277          type crlf
1278          type *,' There is no preparation procedure #'
1279          type 602,' Enter #, or hit ENTER to leave blank:'
1280 590      format (a31,$)
1281 591      format (a35,$)
1282 592      t_prep_proc=' '
1283          accept 252,t_prep_proc
1284          do k = 1,14
1285              if (t_prep_proc(k:k) .ne. ' ')then
1286                  prep_proc = t_prep_proc
1287                  goto 600
1288              end if
1289              prep_proc = ' '           ! default #
1290          end do
1291      end if
1292 600      do i= 1,14
1293          if (anal_proc(i:i) .ne. ' ') go to 650
1294      end do
1295      if (i .ge. 14) then
1296          anal_proc = ' '
1297          if (procedure_flag)then
1298              type *,bell
1299              type 590,' Enter analysis procedure # : '
1300              go to 601
1301          end if
1302          type crlf
1303          type *,' There is no analysis procedure'
1304          type 602,' Enter #, or hit ENTER to leave blank:'
1305 602      format(a38,$)
1306 601      t_anal_proc = ' '

```

```

1307          accept 252,t_anal_proc
1308          do k = 1,14
1309              if (t_anal_proc(k:k) .ne. ' ') then
1310                  anal_proc = t_anal_proc
1311                  goto 650
1312              end if
1313              prep_proc = ' ' ! default #
1314          end do
1315      end if
1316
! To convert 'as-measured' to customer-specific results.

1317      650    new_req = 0
1318      mark = 0
1319      char = '*' ! Will be printed as indicator that data not changed'
1320      if (less_thn .eq.'<' .or. less_thn .eq. '>')go to 660
1321      limit = l_limit
1322      if (customer_limit .ne. 0) limit = c_low_limit
1323      do i = 1,8
1324          if(limit(8:8) .eq.' ')then
1325              limit(2:8) = Limit(1:7)
1326              limit(1:1) = ' '
1327          end if
1328      end do
1329      read(limit,'(f8.5)')xl_limit
1330      read(result,'(f8.3)')r_result
1331      dum = change_data(last_req)
1332      do ind = 1,3      !n,p,3,4 may be in any order
1333      if (dum(ind:ind).eq.'N'.or.dum(ind:ind).eq.'n')goto 651
1334      if (dum(ind:ind).eq.'P'.or.dum(ind:ind).eq.'p')goto 653
1335      if (dum(ind:ind).eq.'3'.or.dum(ind:ind).eq.'4')goto 655
1336      if (dum(ind:ind).eq.' ') go to 670

1337
! *** To convert 'N' to 'NO3'

1338      651    if ( method(1:3).eq.'NO3'.or.method(1:3).eq.'TKN' ) then
1339          factor = 4.4268
1340          r_result = r_result * factor           !N ---> NO3
1341          xl_limit = xl_limit * factor
1342          write (low_limit,'(f8.3)')xl_limit
1343          type *, ' Detection limit = ',low_limit
1344          if (i_blanksub .eq. 1) then
1345              r_blank = r_blank(kl) * factor
1346              r_result = r_result - r_blank
1347              mark = 1 !'mark' is flag indicating blank subtracted
1348          end if
1349          write (a_result,'(f8.3)')r_result
1350          type *,a_result,r_result,result
1351          char = 'C' ! Data were changed
1352      end if
1353      go to 670

1354
! *** To convert 'P' to something else ('factor' is conversion factor)

1355      653    if (method(1:3).eq.'PO4'.or.method(1:3).eq.'TKP') then
1356          r_result = r_result * factor
1357          xl_limit = xl_limit * factor
1358          write(low_limit,'(f8.3)')xl_limit
1359          type *, ' Detection limit = ',low_limit
1360          if (i_blanksub .eq. 1) then
1361              r_blank = r_blank(kl) * factor
1362              r_result = r_result - r_blank
1363              mark = 1
1364          end if
1365          write (a_result,'(f8.3)')r_result

```

```

1366      char = 'C'
1367      end if
1368      go to 670

1369      ! *** To convert 'NH3 results' to 'NH3'.Method determines NH3 as N

1370      655      if (method(1:3) .eq. 'NH3') then
1371          if (c_one .eq.'3' )then
1372              factor = 1.21589
1373              r_result = r_result * factor !N ---> NH3
1374              xl_limit = xl_limit * factor
1375              write (low_limit,'(f8.5)')xl_limit
1376              type 656, ' Detection limit (NH3) = ',low_limit
1377              if (i_blanksub .eq. 1) then
1378                  blanc = r_blank(kl) * factor
1379                  r_result = r_result - blanc
1380                  mark = 1
1381              end if
1382              char = 'C'
1383          end if
1384          format(a25,a8)
1385          if (c_one .eq. '4' )then
1386              factor = 1.28571
1387              r_result = r_result * factor !N ---> NH4
1388              xl_limit = xl_limit * factor
1389              write (low_limit,'(f8.5)')xl_limit
1390              type *, ' Detection limit (NH4) = ',low_limit
1391              if (i_blanksub .eq. 1 ) then
1392                  blanc = r_blank(kl) * factor
1393                  r_result = r_result - blanc
1394                  mark = 1
1395              end if
1396              char = 'C'
1397          end if
1398          write (a_result,'(f8.3)')r_result
1399      end if
1400      670      continue
1401      end do

1402      if (mark .eq. 0 .and. i_blanksub .eq. 1)then
1403          char = '**'
1404          if (in_sample_type .eq. 1) then
1405              r_result = r_result - r_blank(kl)
1406              write (a_result,'(f8.3)')r_result
1407          end if
1408      end if
1409      if (r_result .lt. xl_limit)then
1410          less_thn = '< '
1411          if(in_sample_type.eq.1)lt_count = lt_count + 1
1412          r_result = xl_limit
1413          write (a_result,'(f8.3)')r_result
1414      end if
1415      mark = 0
1416      if(del_sample(j))go to 99

1417      615      format (a8)
1418      6151     format (a,f8.3,f8.3)
1419      620      format (f16.0)
1420      625      format (a8)
1421      mode = ' '
1422      if (method_code(2:5) .eq. '      ') char = '**'
1423      mode(1:1)=char
1424      if (i_blanksub .eq. 1) mode(2:3) = bkgd_subtract(1:2)
1425      if (ic_flag.or.i_blanksub)type*, ' Original result : ',o_result
1426      type *, ' ', sample_number,' ',c_badge_number,' ',method_code,mode,j

```

```

1427      type *, ' ', less_thn,a_result,error,' ',a_units,prep_proc,anal_proc
1428      if (in_sample_type .eq. 1) then
1429          analysis = method
1430          procedure_flag = 0
1431      end if
1432      if (kl .lt. 2) go to 99
1433      if (less_thn .eq. '> ')go to 99
1434      !      type *, ' Storing sample result'
1435      write(16,50) sample_number,c_badge_number,method_code,
1436      1 less_thn,a_result,error,a_units,prep_proc,anal_proc
1437      write(18,50) sample_number, c_badge_number, method_code,
1438      1 less_thn, a_result, error, a_units, prep_proc, anal_proc
1439      type crlf
1440      end if
1441      goto 99
1442      700      continue
1443      ! Insert 'end-of-file' as '$$$'
1444      sample_number = dollars
1445      write(16,50) sample_number, c_badge_number, method_code,
1446      1 less_thn, a_result, error, a_units, prep_proc,anal_proc
1447      write(18,50) sample_number, c_badge_number, method_code,
1448      1 less_thn, a_result, error, a_units, prep_proc,anal_proc
1449      go to 800
1450      50      format (a10/a6/a30/a2/a8/a8/a10/a14/a14 )
1451      99      if (filler(19:26) .eq. 'QuikCalc') go to 6
1452      9099    continue
1453      end do !this is the end of the main sample search loop(index var j)
1454      9100    continue
1455      end do !this is the kl-loop terminator
1456      do i = 1,npos
1457          if (fill_buf(i)(5:5) .eq. 'x') then
1458              kdel=kdel+(kl_pos-2)
1459              type *, ' Deleted : ',fill_buf(i)
1460          end if
1461      end do
1462      filler = fill_buf(42)
1463      if (filler(19:26) .eq. 'QuikCalc') go to 6
1464      if (filler(1:12) .eq. ' End of data') go to 700
1465      800    continue
1466      899    close (unit=15)
1467      close (unit=16)
1468      close (unit=18)
1469      type crlf
1470      if (itrays .lt.1) then
1471          type *, ' No data stored'
1472          type *,bell
1473          go to 8989
1474      end if
1475      if (itrays .lt.2 )then
1476          type *, ' Total vials: ',in_count,' from ',itrays,' tray.'
1477      end if
1478      if (itrays .gt.1) then
1479          type *, ' Total vials: ',in_count,' from ',itrays,' trays.'
1480      end if

```

```

1481      if ( n_outliers .gt. 1 ) type *, '    of these, ',n_outliers,
1482      1 ' were high (not reported)'
1483      if (n_outliers .eq. 1 ) type *, '    of these, ',n_outliers,
1484      1 ' was high (not reported)'
1485      type crlf
1486      type *, '      Standards : ',k_std
1487      type *, '      W-Blanks  : ',k_blank
1488      type *, '      R-Blanks  : ',kr_blank
1489      type *, '      EPA stds  : ',k_epa
1490      type *, '      Pet's    : ',k_pet
1491      type *, '      Other     : ',k_spec
1492      type crlf
1493      isum=0
1494      isum=k_std+k_blank+kr_blank+k_epa+k_pet+k_spec
1495      isum = in_count - isum
1496      type *, '      Samples   : ',isum
1497      type *, '      < detect  : ',lt_count
1498      type *, '      Deleted   : ',kdel,' (includes high results)'
1499      type crlf
1500      do i = 2,kl_pos-1
1501          ipos=index(analyte(i), ' ')
1502          type *, ' ',Analyte(i)(1:ipos), "'s deleted : ",delspec(i)
1503      end do
1504      type *, ' Prepared with fis_parse,version : ',version
1505      898      format (/)
1506      type *,bell,bell,bell
1507      8989     end

1508      ! ****
1509      subroutine read_filler
1510
1511      character*60    filler,blanks
1512      common filler,blanks
1513
1514      888      icount=0
1515      filler = blanks
1516      read (15,27,err=900) filler
1517      27      return
1518      889      continue
1519      27      format(a60)
1520      900      continue
1521
1522      !      type *, ' End on error or end of file'
1523      !      filler(1:12) = ' End of data'
1524      !      return
1525      9000     end!

```

APPENDIX A

PART II. LOGICAL FLOW OF THE PROGRAM

Logical flow of the program is presented in this appendix. Some conventions have been adopted to simplify the format.

- Bold-face print is used for explicit filenames
- The logical IF is also printed in bold-face type
- Italics are used to indicate arbitrary filenames
- Underscored words are the actual variable name used in `fis_parse`.
- Numbers after a GOTO indicate the logic line number;
i.e., the numbers in the left-hand column.
- Numbers in the right-hand column are the text line numbers from the FORTRAN program, `fis_parse.for`.
- Numbers used in the graphical construction of the logic diagram refer to the numbers in the left-hand column

The logical development as presented here is not complete in detail. Rather, it is an attempt to show the programmatic sequence used. Those portions of the program that are sufficiently clear in the original FORTRAN program are not included.

1	SETUP String lengths,variable types, array dimensions	40-70
2	Define COMMON variables	71
3	Define crlf as 'carriage return/line feed'	72
4	ENTER <i>filename</i> [Default = fis.dat]	73-83
5	OPEN file <i>filename</i> . GOTO 4 if file not found	84
6	OPEN file 'tempo1.dat' as backup file	86
7	OPEN file 'file_transfer.dat' as primary data file	89
8	INITIALIZE variables	92-122
9	BEGIN READ one line from <i>filename</i>	124
10	TEST line GOTO 9 if all characters blank	125
11	TEST line GOTO 355 if ' End of data' message	126
12	TEST line GOTO 9 if beginning of report not found	127
13	READ first line of report REPEAT this line if blanks	130
14	TEST line GOTO 355 if ' End of data' message	132
15	INCREMENT tray counter	139
16	READ report date and report time/re-format	140-151
17	CLEAR requisition number array & deletion info arrays	156-160
18	READ line	162
19	TEST line if 1st char is 'T' char's 44-52 = sequence #	163
20	TEST line if 1st char not 'M'(ethod) GOTO 18	164
21	SET <u>method</u> = char's 9-32	165
22	JUSTIFY <u>method</u> to left	166-170
23	TEST line if '/' found then there is more than one	172-187
24	method. Save methods as <u>multi-method</u>	
25	TEST <u>method</u> if is not the same as previous tray,	195-198
26	clear procedure #'s	
27	SET <u>badge number</u> = <u>char's 34-56</u>	200
28	TEST <u>badge number</u> to find position of ':'--the start	201-202
29	of the number	
30	TEST following 8 char's; if correct GOTO 32	202-208
31	INPUT <u>badge number</u> (from KBD), GOTO 30	206
32	JUSTIFY <u>badge number</u> to right	210-214
33	TEST <u>badge number</u> if not all numerals GOTO 31	216-223
34	READ line (Find Customer Request Numbers)	225-257

35 {Note: Tray Comments area has 255 chars which are used
 36 to enter customer request numbers. Numbers are separated
 37 with ';'. Imbedded blanks not allowed. A request number
 38 may have 1-11 char's.)
 39 TEST line if blank GOTO 34 225-226
 40 TEST line if 1st 14 char's not 'Tray Comments'
 41 227
 41 GOTO 14
 42 CLEAR previous request numbers 231-234
 43 SET sequential char's on line = char 237
 44 TEST a char from current line 238-257
 45 if char is numeral and not a ';', add char to
 46 req_number; GOTO 43, else
 47 if char is blank GOTO 34, else
 48 if char is ';', increment request number counter,
 49 start new requisition number;
 50 GOTO 43
 51 READ line if blanks REPEAT else 239-240
 52 if end of line and char not blank then 248-255
 53 READ line if blank REPEAT
 54 if char's 4-9 = 'Anal' GOTO 56 250-254
 55 else GOTO 43
 56 TEST char's 17-24 if blank Warn Operator, GOTO 12 261-264
 57 SET Number of Analytes = 4 266-274
 58 analyte #1 = char's 17-45
 59 analyte #2 = char's 17-23
 60 analyte #3 = char's 28-34
 61 analyte #4 = char's 39-45
 62 TEST analytes if blank, Decrement Number of Analytes 275-279
 63 PROCESS reg_number: Remove trailing ';' or blank 281-307
 64 Prefix with lab code letters
 65 Display Request Numbers
 66 READ line if blank, REPEAT 309-310
 67 if char's 19-23 = "QuikC" GOTO 13 311
 68 if char's 1-3 = "Cup" then 312
 69 CLEAR old units and 321-328
 70 SET units #2 = char's 18-23 313-320
 71 units #3 = char's 29-34
 72 units #4 = char's 40-45
 73 units #5 = char's 51-56
 74 JUSTIFY units to left 321-328
 75 {Note: In the next section the operator selects which samples and
 76 analytes to report and which customer requests to process.}
 77 INITIALIZE variables 343-357
 78 DISPLAY "New Tray--hit ENTER to continue or '\$' to skip 358
 79 TEST KBD [keyboard] if KBD = \$ GOTO 12 361
 80 if KBD not = \$ GOTO 82 362

```

81      {Note:Select analytes to report}

82      INCREMENT      analyte counter

83      TEST  analyte counter  if count =1 GOTO 97      363-400
84          if count >1

85      DISPLAY  "Select analytes to report"

86      DISPLAY  Table of analyte #'s and analytes

87      DISPLAY  "Hit ENTER to report all analytes,or enter the
88          numbers of analytes you want to report."

89      TEST    KBD  if blank GOTO 97      382
90          if not valid GOTO 87      390

91      CONVERT  KBD ASCII to Real #

92      TEST    KBD(real #)  if not valid # GOTO 87      392
93          if valid

94      DISPLAY  "Enter next number;terminate with      396
95          ENTER only". GOTO 89

96      {Note:Select customer request numbers to process or omit}

97      TEST    n requests  if n requests =1 GOTO 129      403-546
98          if n requests >1

99      DISPLAY  "Enter $ if you want to process data by      407
100         request,hit ENTER to process all requests"

101     TEST    KBD  if KBD = blank GOTO 129      412
102         if KBD = $

103     DISPLAY  "OPTION: S(ave) or D(elete) ?"      414

104     DISPLAY  "If you save one or more requests, those      416-419
105         not deleted will be processed,
106         If you D(elete) one or more requests,
107         those not deleted will be processed"

108     DISPLAY  req number's      423-428

109     DISPLAY  "please type S or D"      430

110     CLEAR   old delete flags      432-437

111     TEST    KBD  if KBD = S, msg = save      439-443
112         if KBD = D, msg = delete      444-448

113     DISPLAY "Enter the request #(s)'s +msg"      454-456
114         (an example)
115         "Hit ENTER to process all requests"

116     TEST    KBD  if KBD = blank GOTO 129      458
117         if KBD not valid GOTO 113      459-472
118         if KBD valid

119     COMPARE  Deletion flag number with req_number number      478-496
120         if match, mark request number for
121             deletion

```

122	TEST	# of requests for deletion if > # requests GOTO 113	499-501
123			
124	TEST	request numbers for duplicates if duplicate #'s GOTO 113	514-527
125			
126	TEST	if # does not exist GOTO 113	529-533
127	TEST	# deleted minus Total requests if = 0, GOTO 9	544
128			
129	DISPLAY	"Is it OK to proceed?" "Hit ENTER if OK; anything else to change"	548
130			
131	TEST	KBD if not blank, GOTO 78	552
132		INCREMENT trays processed	555
133		(Note: The sample data section of the file will be processed once more than the number of analytes found. On the first pass, count vials on tray, identify reagent blanks, store each line of the report, display the lines as they appear in the report)	
134			
135			
136			
137			
138		SET pass counter = 0, line counter = 0	
139		INCREMENT pass counter	
140		INCREMENT line counter	
141	TEST	pass number if not = 1 GOTO 188	595
142	READ	line if blank, REPEAT	596-597
143	TEST	line if char's 1-12 = 'End of data', GOTO 146	598
144			
145	TEST	line if char's 19-26 equal "QuikCalc", then if more than one blank found GOTO 150	601
146			
147			
148			
149			
150			
151	DISPLAY	Cup number and data on line	
152	STORE	line of data	692
153	TEST	1st char of sample # if 'b'(vial is a blank) 694	
154		INCREMENT blank counter	695
155		SET <u>blanko</u> = value of blank	698
156	TEST	<u>blanko</u> if < min detectable <u>blanko</u> = '0000.000' if => min detectable	700
157			
158	JUSTIFY	to right	703-708
159	CONVERT	to Real #	709
160	CALCULATE	mean value of blanks found for each analyte	711-715

161	DISPLAY instructions for selecting, modifying, deleting or entering new values for blanks;	605-671
163	DISPLAY "To select blank result to use, enter A,D,M,or N"	608-609
165	DISPLAY analyte and values of reagent blanks	611-615
166	TEST KBD if not valid, GOTO 161	672-675
167	TEST KBD if 'A', msg = "use", flag = 1	620-621
168	if 'D', msg = "delete", flag = 2	623-626
169	TEST flag if <1, GOTO 180	627
170	DISPLAY "please enter the number of the blank to +msg"	628
172	READ KBD	629
173	JUSTIFY KBD entry to right	630-635
174	TEST KBD if not valid input, GOTO 170	636-638
175	CONVERT KBD entry to INTEGER	639
176	TEST flag if '1',	
177	SET blank value = selected value	640
178	TEST flag if '2',	641-649
179	RECALCULATE mean without this blank , GOTO 161	
180	TEST KBD if 'M',	653-656
181	SET blank value = mean, flag = 3, GOTO 185	
182	TEST KBD if 'N'	657-666
183	ENTER value of blank to use,	
184	JUSTIFY to right	
185	CONVERT blank value to Real #	670
186	GOTO 139	
187	{Note: Second and subsequent passes begin here.}	
188	READ one line of file created during first pass	735
189	TEST first char of sample number area (char's 5-15)	748
190	{Note: Samples begin with a numeral. Only samples are 191 to be processed for entry into Analis. Other types of 192 materials are identified by code, the report line 193 displayed, and the number of occurrences of each type 194 tallied. This outline shows the processing to which 195 samples only are subjected.}	

196	SET	Sample type = 1	747
197	TEST	Sample type if not = 1, GOTO 140	794
198		*	
199	(Note: Three possibilities are considered in the next section: 1)New request number as indicated by the dash in position 7 of the sample number,2)sub-sample of the current request,3)a duplicate or sample for which there was a sampling error.)		
204	TEST	<u>sample number</u> if char 7 = '-',	810
205	TEST	first six char's of <u>sample number</u> if numerals GOTO 216	811-813
207	DISPLAY	"Present sample:(data line)"	815
208	DISPLAY	"Enter correct sample #, 's' to omit result, or 'd' to delete entire sample"	818
209			
211	TEST	KBD if char = 'd', increment samples deleted; place an 'x' in first char of sample number in file; GOTO increment line #	820-825
214	TEST	KBD if char = 's', increment results deleted; GOTO increment line #	826-829
215			
216	SET	- <u>new req</u> = 1, increment req #, - <u>root sample id</u> = 1st 6 char's of <u>sample number</u>	832
217			834
218			
219		- <u>ident(8-11)</u> = char's 12-15 on line GOTO 226	836
220			
221	TEST	'delete sample flag' if TRUE, GOTO 140	842
222			
223	(Note: The next three chars are the sub-sample #, to be appended to the <u>root sample id</u> if they are numerals. They may be on the same or next line.)		
226	TEST	<u>ident(8-11)</u> Left justify,filling with blanks; then Right justify adding leading zero's as required	851-867
227			
228			
229	TEST	<u>ident(8-10)</u> if all numerals,GOTO 240	869-875
230	DISPLAY	"Sub-sample # in error;now: <u>ident</u>	872
231	DISPLAY	"Enter correct sub-sample #,'s' to skip, or 'd' to delete sample"	874
232			
233	SET	<u>ident(8-10)</u> = answer	876
234	TEST	<u>ident</u> if any char = 'd', place an 'x' in 1st char position of sample number; increment samples deleted; GOTO increment line number	877-889
235			
236			
237			
238			
239			

240	SET	<u>serial number</u> = <u>ident(8-10)</u>	890	
241	{Note: Assemble the full sample number}			
242	TEST	<u>new reg</u> if = 1, replace sample number in file	900	
243	TEST	if char's 1-3 of <u>ident</u> = char's 1-3 of	901	
244		<u>root sample id</u> , GOTO 251		
245		if char's 1-3 of <u>ident</u> not = char's 1-3 of		
246		<u>root sample id</u> ,		
247	SET	<u>sample number(1-3)</u> = <u>serial number</u>	902-903	
248		<u>sample number(4-11)</u> = blank		
249	STORE	<u>sample number</u>		
250	{Note: Possibility #3}			
251	TEST	<u>sample number</u> if any char = 'x' or '+'	906-915	
252		GOTO 140		
253	{Note: The next section produces a customer-specific			916-1205
254	report.}			
255	TEST	if not new analyte, GOTO 258	920-933	
256		if new analyte,		
257	SET	new request # to first request number		
258	TEST	if delete this request TRUE, GOTO 261		
259	TEST	if not new request, GOTO 305		
260		if new request,		
261	DISPLAY "SELECT OPTIONS" for request number: + <u>req number</u>			936
262	DISPLAY "Enter customer value for detection limit;			940
263	otherwise,ENTER"			
264	TEST	KBD if response not valid, GOTO 261	942-947	
265		if valid,		
266	CONVERT	response to Real number and replace limit of	948	
267		detection with this number		
268	{Note: In the next section, unwanted data for a sample			959-1007
269	may be eliminated from report.}			
270	DISPLAY "Do you want to eliminate any results?"			962
271	TEST	KBD if no, GOTO 282	964	
272		if yes,		
273	DISPLAY "Enter the cup #'s of the results to delete;			966
274		end input with blank (ENTER)"		
275	TEST	KBD if not valid response, GOTO 273	969-994	
276		if valid,		
277	SET	delete flag = TRUE	995	
278	DISPLAY list of results to be deleted			999-1007
279	DISPLAY "Are there any changes?"			1009

280	TEST	KBD	if yes, GOTO 270 if no,	1009-1018
282	(Note: In the following sections, setups for nitrate, phosphate, and ammonia are treated separately, in order. Internal documentation should be adequate to understand the logical flow of the program in these sections; these steps will be omitted here.)			1024-1170
287	DISPLAY "Request #: + <u>reg number</u> "			1174
288	DISPLAY " You have selected the following options:			1176
289	(Note: Here the program makes use of flags that were set in the setup section to assist in displaying a list of options selected. The user has the option of accepting or changing the selections made. The programming is self- explanatory.)			
294	TEST	if there is one or more reagent blanks and if the option of subtracting the blank was selected, the user is asked:		1192
297	DISPLAY "Enter 'c' to subtract reagent blank; ENTER = no blank correction"			1194
299	DISPLAY "Hit ENTER if (all choices) OK; any number to change"			1200
301	TEST	KBD	if not blank, GOTO 261 if blank(no changes),	1202
303	(Note: Continue examination of data report line at results position.)			
305	TEST	results area	if char not = '<' AND char not = 'high', GOTO 312	1212
308	SET	<u>result</u>	= result char's	1244
309	JUSTIFY	<u>result</u>	to right	
310	SET	<u>o_result</u>	= <u>result</u> (save for display as 'original data' later)	1253
312	TEST	'delete sample' flag	if TRUE, GOTO 331	1259
313	TEST	'procedure' flag	if NOT TRUE, GOTO 316 (true = change #'s)	1260
315	CLEAR	procedure numbers		1261-1263
316	TEST	same analyte and requisition # as previous Sample? TRUE, GOTO 331		1264
318	DISPLAY "Enter Preparation Procedure #"			1274
319	TEST	preparation procedure # if not blank,GOTO 323 if blank,		1272-1291
321	DISPLAY "There is no preparation procedure #; enter the #, or hit ENTER to leave blank"			
323	DISPLAY "Enter analysis procedure #"			1299

```

324 TEST analysis procedure # if not blank,GOTO 331 1300
325 if blank,
326 DISPLAY "There is no analysis procedure #;
327 enter the #, or hit ENTER to leave blank"
328 TEST convert to another species flag 1332-1336
329 if NOT TRUE, GOTO 349
330 if TRUE,
331 (Note: In the following section, conversion
332 to another species is made and results corrected for
333 reagent blank if previously requested. The logical flow
334 is illustrated for only one generic species. That species
335 could be either nitrogen(as nitrate or ammonia) or
336 phosphorous. It is also assumed that quantities that
337 will be used in arithmetic operations are first converted
338 to real numbers.)
339 TEST analyte if nitrate, GOTO nitrate 1332-1336
340 if ammonia, GOTO ammonia
341 if phosphate, GOTO phosphorous
342 generic procedure
343 SET result = result * conversion factor
344 detection limit = detection limit * conversion
345 factor
346 TEST 'subtract blank' flag if not TRUE, GOTO 349 1317-1383
347 if TRUE,
348 SET result = result - blank
349 TEST result if > detection limit, GOTO 355 1409-1414
350 if < detection limit,
351 SET result = detection limit
352 TEST delete sample flag if TRUE, GOTO 140
353 (line counter)
354 if NOT TRUE, GOTO 355
355 SET sample number = '$$$' (end-of-file marker
356 for Analis)
357 DISPLAY sample information 1425-1423
358 STORE sample data that will be transferred to Analis 1434-1440
359 TEST line counter if not = # vials, GOTO 357
360 SET line counter = 0
361 GOTO 139
362 GOTO 140 1441
363 ****
364 SUBROUTINE
365 The subroutine has two functions:
366 1) It is here that a line of data is read
367 from the original record.

```

368 2) The end of the original record is signaled
369 by an attempt to read past the end of the file.
370 The error is trapped by the READ statement, and
371 the message 'End of data' substituted for the
372 line returned to the calling program.

373 (Note: The 'End of data' message is stored in location 42--
374 a non-existent vial position. After processing of a tray is
375 complete, this location is read first to determine if it holds
376 the 'End of data' message.)

THIS PAGE LEFT BLANK INTENTIONALLY

APPENDIX B
SAMPLE DATA REPORT FROM FIS

This listing copied via ETHERNET (Digital Equipment Corp.) from the VAX 8300 to drive 'a' on a personal computer. It has been compared with the original data and found to be uncorrupted. The data file is FIS13.DAT. The working copy from which the data of this appendix were derived resides in the VAX computer. The trays included were selected to illustrate most of the features of FIS_PARSE.

```
1          QuikCalc II Sample Report
2
3          Tray ID: #2           5/ 9/1988 15:42
4          Method: NH3 salicylate Reference: 8805090J
5
6
7          Tray Comments: 9718;9793;
8
9          Analyte -> NH3/N
10         Base Correction Yes
11         Technique Area
12
13         ----- Calibration -----
14         Seg 1 C.C.    0.99971 .
15         Seg 2 C.C.    0.999672 .
16
17
18         Analyte -> NH3/N
19         Cup Sample I.D.    UG/ML      Dil
20
21         1 h2O        0.002      1.00
22         2 s 0.050    0.047      1.00
23         3 s 0.100    0.098      1.00
24         4 880331-293 0.226      1.00
25         5 880420-16   0.073      1.00
26         6 17         0.072      1.00
27         7 18         0.048      1.00
28         8 19         0.050      1.00
29         9 20         0.064      1.00
30         10 21        0.059      1.00
31         11 22        0.047      1.00
32         12 23        0.054      1.00
33         13 24        0.073      1.00
34         14 25        0.102      1.00
35         15 26        0.049      1.00
36         16 27        0.015      1.00
37         17 28        0.018      1.00
38         18 29        0.039      1.00
39         19 30        0.058      1.00
```


92 25 25-2 0.086 0.280 4.00
93 26 s 0.400 0.400 0.404 A- 1.00
94 27 blk 0.014 < x.xx
95 28 blk < x.xx 0.002
96 QuikCalc II Sample Report
97 5/11/1988 15:33
98 Tray ID: #6 Reference: 8805110H
99 Method: NH3 salicylate Operator: 13164
100
101
102 Tray Comments: 9793;9751;9752;
103
104 Analyte -> NH3/N
105 Base Correction Yes
106 Technique Area
107
108 ----- Calibration -----
109 Seg 1 C.C. 0.99966 .
110 Seg 2 C.C. 0.99205 .
111
112
113 Analyte -> NH3/N
114 Cup Sample I.D. UG/ML Dil
115
116 1 H2O 0.006 1.00
117 2 s0.050 0.042 1.00
118 3 s 0.100 0.100 1.00
119 4 Pet-3 55.001 A- 100.00
120 5 Pet-4 156.999 A- 262.50
121 6 pet-1 25.067 200.00
122 7 Pet-2 210.689 A- 500.00
123 8 880420-56 0.019 1.00
124 9 57 0.017 1.00
125 10 58 0.020 1.00
126 11 59 0.020 1.00
127 12 60 0.022 1.00
128 13 61 0.029 1.00
129 14 62 0.046 1.00
130 15 63 0.048 1.00
131 16 64 0.020 1.00
132 17 880411-38 0.004 1.00
133 18 QNS 39 0.003 1.00
134 19 40 0.010 1.00
135 20 880411-41 0.116 1.00
136 21 42 0.618 A- 1.00
137 22 43 0.186 1.00
138 23 44 0.089 1.00
139 24 45 0.202 1.00
140 25 46 0.137 1.00
141 26 47 0.017 1.00
142 27 48 0.495 A- 1.00
143 28 49 0.025 1.00

144 29 50 0.354 A- 1.00
 145 30 51 0.540 A- 1.00
 146 31 s 0.400 0.407 A- 1.00
 147 QuikCalc II Sample Report
 148 5/11/1988 10: 8
 149 Tray ID: #1 Reference: 8805110C
 150 Method: TKN/TKP 5/10/88 Operator: 13164
 151
 152
 153 Tray Comments: 9626;

154
 155 Analyte -> TKP TKN
 156 Base Correction Yes Yes
 157 Technique Area Area
 158
 159 ----- Calibration -----
 160 Seg 1 C.C. 0.99824 . 0.99983 .
 161 -----

162
 163 Analyte -> TKP TKN
 164 Cup Sample I.D. UG/ML UG/ML Dil
 165
 166 1 H2O 0.018 < x.xx D- 1.00
 167 2 s 0.100 0.093 0.099 1.00
 168 3 s 0.200 0.190 A- 0.197 1.00
 169 4 s 0.400 0.401 0.403 A- 1.00
 170 5 EPA284-4 29.780 165.500 A- 500.00
 171 6 EPA 30.884 166.363 A- 500.00
 172 7 880310-26-1 0.143 0.335 4.00
 173 8 26-2 0.092 0.295 4.00
 174 9 27 0.100 0.295 4.00
 175 10 28 0.126 0.336 4.00
 176 11 29 0.102 0.271 4.00
 177 12 30 0.120 0.239 4.00
 178 13 31 0.091 0.171 4.00
 179 14 32 0.076 0.164 4.00
 180 15 33 0.084 0.255 4.00
 181 16 34 0.080 0.203 4.00
 182 17 35 0.083 0.227 4.00
 183 18 36 0.089 0.181 4.00
 184 19 37 0.123 0.182 4.00
 185 20 38 0.110 0.232 4.00
 186 21 s 0.200 0.188 A- 0.194 1.00
 187 22 39 0.091 0.240 4.00
 188 23 40 0.147 0.148 4.00
 189 24 41 0.068 0.269 4.00
 190 25 BLK 0.025 < x.xx D- 1.00
 191 26 s 40ng 36.103 38.784 A- 100.00
 192 27 EPA486-2 130.720 497.250 A- 1050.00
 193 28 43 0.142 0.490 4.00
 194 29 47 0.128 0.750 4.00
 195 30 s 0.400 0.401 0.402 A- 1.00

196 QuikCalc II Sample Report
 197 5/11/1988 12:16
 198 Tray ID: #2 Reference: 8805110D
 199 Method: TKN/TKP 5/10/88 Operator: 13164
 200
 201
 202 Tray Comments: 9626;

203 Analyte -> TKP TKN
 204 Base Correction Yes Yes
 205 Technique Area Area
 206

207 -----Calibration-----
 208 Seg 1 C.C. 0.99789 . 0.99918 .
 209

	Analyte -> TKP	TKN	
Cup	Sample I.D.	UG/ML	UG/ML
215	1 H2O	0.021	0.011
216	2 s 0.100	0.089	0.097
217	3 s 0.200	0.188	0.192
218	4 880310-48	0.103	0.321
219	5 49	0.124	0.102
220	6 50	0.090	0.092
221	7 51	0.116	0.087
222	8 52-1	0.095	0.021
223	9 52-2	0.117	0.079
224	10 53	0.100	0.051
225	11 54	0.112	0.076
226	12 55	0.092	0.002
227	13 56	0.102	0.002
228	14 57	0.091	0.241
229	15 58	0.090	< x.xx D- 4.00
230	16 59	0.091	0.617
231	17 60	0.090	0.453
232	18 61	0.090	0.172
233	19 BLK	0.023	< x.xx D- 1.00
234	20 s 40ng	36.532	35.662 A- 100.00
235	21 EPA486-2	120.029	468.453 A- 1050.00
236	22 66	0.080	0.047
237	23 67-1	0.112	0.100
238	24 67-2	0.135	0.092
239	25 68	0.136	0.098
240	26 69	0.103	0.068
241	27 70	0.173	0.134
242	28 71	0.132	0.177
243	29 72	0.178	0.151
244	30 s 0.400	0.401	0.406 A- 1.00

245 QuikCalc II Sample Report
 246 5/11/1988 13:14
 247 Tray ID: #3 Reference: 8805110E

248 Method: TKN/TKP 5/10/88 Operator: 13164

249

250

251 Tray Comments: 9626;

252

253 Analyte -> TKP TKN
254 Base Correction Yes Yes
255 Technique Area Area

256

257 ----- Calibration -----
258 Seg 1 C.C. 0.99747 . 0.99989 .
259 -----

260

261 Analyte -> TKP TKN
262 Cup Sample I.D. UG/ML UG/ML Dil
263
264 1 s 0.100 0.088 0.100 1.00
265 2 s 0.200 0.186 0.199 1.00
266 3 H2O 0.007 0.003 1.00
267 4 880310-73 0.098 0.074 4.00
268 5 74 0.106 0.358 4.00
269 6 Pet-3 5.935 HIGH A- 50.00
270 7 Pet-3 5.436 54.850 A- 100.00
271 8 Pet-4 HIGH HIGH A- 50.00
272 9 Pet-4 42.677 HIGH A- 100.00
273 10 BLK 0.006 < x.xx D- 1.00
274 11 s 20ng 19.628 A- 19.215 100.00
275 12 s 40ng 36.799 38.211 A- 100.00
276 13 EPA486-2 129.357 479.228 A- 1050.00
277 14 s 0.400 0.396 0.401 A- 1.00
278 QuikCalc II Sample Report
279 5/11/1988 14:44

280 Tray ID: #5

Reference: 8805110G

281 Method: NH3 salicylate

Operator: 13164

282

283

284 Tray Comments: 9793;

285

286 Analyte -> NH3/N
287 Base Correction Yes
288 Technique Area

289

290 ----- Calibration -----
291 Seg 1 C.C. 0.99966 .
292 Seg 2 C.C. 0.99644 .
293 -----

294

295 Analyte -> NH3/N
296 Cup Sample I.D. UG/ML Dil
297

298 1 H2O 0.002 1.00
 299 2 s 0.050 0.046 1.00
 300 3 s 0.100 0.101 1.00
 301 4 Pet-3 HIGH A- 100.00
 302 5 Pet-4 156.545 A- 262.50
 303 6 Pet-1 26.789 200.00
 304 7 Pet-2 213.605 A- 500.00
 305 8 H2O < x.xx D- 1.00
 306 9 880420-37 0.018 1.00
 307 10 38 0.044 1.00
 308 11 39 0.037 1.00
 309 12 40 0.059 1.00
 310 13 41 0.078 1.00
 311 14 42 0.045 1.00
 312 15 43 0.053 1.00
 313 16 44 0.092 1.00
 314 17 45 0.044 1.00
 315 18 46 0.079 1.00
 316 19 47 0.106 1.00
 317 20 48 0.043 1.00
 318 21 49 0.033 1.00
 319 22 50 0.039 1.00
 320 23 51 0.084 1.00
 321 24 52 0.008 1.00
 322 25 53 0.022 1.00
 323 26 54 0.025 1.00
 324 27 55 0.018 1.00
 325 28 s0.400 0.407 A- 1.00

QuikCalc II Sample Report

5/12/1988 9:37

326 Tray ID: #1 Reference: 8805120B
 327 Method: NH3 salicylate Operator: 13164

332 Tray Comments: 9753;9754;

333 Analyte -> NH3/N
 334 Base Correction Yes
 335 Technique Area

----- Calibration -----

336 Seg 1 C.C. 1.00000 .
 337 Seg 2 C.C. 0.99932 .

342 Analyte -> NH3/N
 343 Cup Sample I.D. UG/ML Dil
 344

345 1 H2O < x.xx D- 1.00
 346 2 s 0.050 0.050 1.00
 347 3 s 0.100 0.101 1.00
 348 4 s 0.200 0.196 1.00

350 5 EPA284-4 173.898 A- 500.00
351 6 EPA 172.215 A- 500.00
352 7 880411-52 0.004 1.00
353 8 53 0.001 1.00
354 9 54 0.009 1.00
355 10 55 0.002 1.00
356 11 56 0.001 1.00
357 12 57 0.002 1.00
358 13 58 0.002 1.00
359 14 59 < x.xx D- 1.00
360 15 60 < x.xx D- 1.00
361 16 61 0.002 1.00
362 17 62 < x.xx D- 1.00
363 18 63 0.002 1.00
364 19 64 0.008 1.00
365 20 880411-65 0.008 1.00
366 21 66 0.027 1.00
367 22 67 0.000 1.00
368 23 68 0.004 1.00
369 24 69 0.004 1.00
370 25 70 0.005 1.00
371 26 71 0.002 1.00
372 27 72 0.001 1.00
373 28 73 0.007 1.00
374 29 74 0.009 1.00
375 30 75 0.006 1.00
376 31 s 0.400 0.404 A- 1.00

QuikCalc II Sample Report

5/12/1988 15:21

Reference: 8805120H

Operator: 13164

377 Tray ID: #6
378 Method: NH3 salicylate

382 383 Tray Comments: 9785;9786;

384 Analyte -> NH3/N
385 Base Correction Yes
386 Technique Area

388 ----- Calibration -----
389 Seg 1 C.C. 0.99979 .
390 Seg 2 C.C. 0.25747 ?
392 -----

393 ----- Calibration -----
394 Seg 1 C.C. 0.99966 .
395 Seg 2 C.C. 0.98475 ?
397 -----

398 Analyte -> NH3/N
399 Cup Sample I.D. UG/ML Dil
400

401
402 1 H2O 0.008 1.00
403 2 s 0.050 0.056 1.00
404 3 s 0.100 0.118 1.00
405 4 880419-55 0.083 1.00
406 5 56 0.087 1.00
407 6 57 0.104 1.00
408 7 58 0.140 1.00
409 8 59 0.162 1.00
410 9 60 0.040 1.00
411 10 61 0.172 1.00
412 11 62 0.165 1.00
413 12 63 0.231 1.00
414 13 64 0.032 1.00
415 14 880419-65 0.310 A- 1.00
416 15 66 0.315 A- 1.00
417 16 67 0.324 A- 1.00
418 17 68 0.314 A- 1.00
419 18 69 0.278 A- 1.00
420 19 70 0.296 A- 1.00
421 20 71 0.301 A- 1.00
422 21 72 0.360 A- 1.00
423 22 73 0.368 A- 1.00
424 23 74 HIGH A- 1.00
425 24 75QNS 0.019 1.00
426 25 76 0.012 1.00
427 26 77 0.013 1.00
428 27 78 0.012 1.00
429 28 79 0.015 1.00
430 29 84 0.092 1.00
431 30 85 0.075 1.00
432 31 s 0.400 0.419 A- 1.00

QuikCalc II Sample Report

5/12/1988 10:23

Tray ID: #2 Reference: 8805120C
Method: NH3 salicylate Operator: 13164

439 Tray Comments: 9754;

440
441 Analyte -> NH3/N
442 Base Correction Yes
443 Technique Area

444
445 ----- Calibration -----
446 Seg 1 C.C. 0.99996 .
447 Seg 2 C.C. 0.99849 .

449
450 Analyte -> NH3/N
451 Cup Sample I.D. UG/ML Dil
452

453	1 H2O	0.006	1.00
454	2 s 0.100	0.102	1.00
455	3 s 0.200	0.191	1.00
456	4 880411-76	0.032	1.00
457	5 77	0.005	1.00
458	6 78	0.002	1.00
459	7 79	0.003	1.00
460	8 80	0.015	1.00
461	9 81	0.007	1.00
462	10 82	0.005	1.00
463	11 83	0.033	1.00
464	12 84	0.007	1.00
465	13 85	0.029	1.00
466	14 86	0.005	1.00
467	15 87	0.007	1.00
468	16 88	0.009	1.00
469	17 89	0.021	1.00
470	18 90	0.005	1.00
471	19 91	0.012	1.00
472	20 92	0.010	1.00
473	21 93	0.007	1.00
474	22 94	0.004	1.00
475	23 95	0.011	1.00
476	24 96	0.006	1.00
477	25 s 0.200	0.197	1.00
478	26 s 0.400	0.409 A-	1.00

QuikCalc II Sample Report

5/12/1988 12:38

Reference: 8805120D

Operator: 13164

481 Tray ID: #3
 482 Method: NH3 salicylate

484
 485 Tray Comments: 9755;

486
 487 Analyte -> NH3/N
 488 Base Correction Yes
 489 Technique Area

490
 491 ----- Calibration -----
 492 Seg 1 C.C. 0.99986 .
 493 Seg 2 C.C. 0.99450 .

495
 496 Analyte -> NH3/N
 497 Cup Sample I.D. UG/ML Dil
 498
 499 1 H2O 0.006 1.00
 500 2 s 0.050 0.048 1.00
 501 3 s 0.100 0.103 1.00
 502 4 s 0.200 0.198 1.00
 503 5 880411-99 0.007 1.00
 504 6 100 0.008 1.00

505	7	101	0.008	1.00
506	8	102	0.014	1.00
507	9	103	0.009	1.00
508	10	104	0.051	1.00
509	11	105	0.017	1.00
510	12	106	0.007	1.00
511	13	107	0.011	1.00
512	14	108	0.007	1.00
513	15	109	0.010	1.00
514	16	110	0.047	1.00
515	17	111	0.008	1.00
516	18	112	0.016	1.00
517	19	113	0.004	1.00
518	20	114	0.009	1.00
519	21	115	0.010	1.00
520	22	116	0.009	1.00
521	23	117	0.011	1.00
522	24	118	0.064	1.00
523	25	119	0.010	1.00
524	26	120	0.008	1.00
525	27	121	0.011	1.00
526	28	122	0.010	1.00
527	29	123	0.009	1.00
528	30	124QNS	0.007	1.00
529	31	s 0.400	0.406 A-	1.00
530				

THIS PAGE LEFT BLANK INTENTIONALLY

APPENDIX C RUN-TIME DIALOG

This appendix shows the dialog between operator and computer while running FIS_PARSE with the input data file, FIS13.DAT. Operator responses are underlined.

```
1      Default filename is 'fis.dat'  
2      Enter new filename, or hit ENTER to use default  
3      fis13.dat  
  
4      NH3 salicylate      : analysis performed on FIS 880509 1542  
5      Sequence # (ref): 8805090J  
  
6      Request Numbers:  
7          EAL9718      EAL9793  
8          Total requests =      2  
9          New tray-- hit ENTER to continue, or '$' to skip tray  
  
10     Enter '$' if you want to process data by request #  
11     Hit ENTER to process all requests  
  
12     Is it OK to proceed?  
  
13     Hit ENTER if OK; anything else to change  
  
14     Cup #    1 h20      0.002      1.00  
15     Cup #    2 s 0.050    0.047      1.00  
16     Cup #    3 s 0.100    0.098      1.00  
17     Cup #    4 880331-293   0.226      1.00  
18     Cup #    5 880420-16   0.073      1.00  
19     Cup #    6 17       0.072      1.00  
20     Cup #    7 18       0.048      1.00  
21     Cup #    8 19       0.050      1.00  
22     Cup #    9 20       0.064      1.00  
23     Cup #   10 21       0.059      1.00  
24     Cup #   11 22       0.047      1.00  
25     Cup #   12 23       0.054      1.00  
26     Cup #   13 24       0.073      1.00  
27     Cup #   14 25       0.102      1.00  
28     Cup #   15 26       0.049      1.00  
29     Cup #   16 27       0.015      1.00  
30     Cup #   17 28       0.018      1.00  
31     Cup #   18 29       0.039      1.00  
32     Cup #   19 30       0.058      1.00  
33     Cup #   20 31       0.027      1.00  
34     Cup #   21 32       0.039      1.00  
35     Cup #   22 33       0.041      1.00  
36     Cup #   23 34       0.066      1.00  
37     Cup #   24 35       0.029      1.00  
38     Cup #   25 36       0.038      1.00  
39     Cup #   26 37       0.022      1.00  
40     Cup #   27 38       0.047      1.00  
41     Cup #   28 s 0.400    0.396 A-    1.00  
  
42     Enter detection limit for NH3/N method.  
43     .001  
44     :water blank & result :  0.002  
45     :standard & result :  0.050  0.047  
46     :standard & result :  0.100  0.098
```

```

47      SELECT OPTIONS -- Request # : EAL9718
48      Enter customer value for detection limit;otherwise,ENTER.
49      .02
50      Do you want to eliminate any results?<y=yes,ENTER=no>
51      Enter '3' to convert 'N' to 'NH3' :
52      Enter '4' to convert 'N' to 'NH4' : 3
53      Report ammonia as [NH3 = default] :
54      Change Procedure #'s ? <y = yes;ENTER = no>y

55      Request #:EAL9718
56      You have selected the following options:
57          Convert N to NH3
58          Analysis Name      : NH3
59          Preparation Procedure # : To be changed
60          Analytical Procedure # : To be changed
61          Hit ENTER if OK; any number or letter to change :
62          Enter preparation procedure # : N1347
63          Enter analysis procedure # : EAL-fis-166
64          Detection limit (NH3) = 0.02432   Calcd. 0.024318
65          Original result : 0.226
66          880331-293 13164 NH3           C      4
67          0.275      UG/ML    N1347     EAL-fis-166
68          Calcd: 0.027479
69          SELECT OPTIONS -- Request # : EAL9793
70          Enter customer value for detection limit;otherwise,ENTER.
71          .02
72          Do you want to eliminate any results?<y=yes,ENTER=no>
73          Enter '3' to convert 'N' to 'NH3' :
74          Enter '4' to convert 'N' to 'NH4' : 4
75          Report ammonia as [NH4 = default] :
76          Change Procedure #'s ? <y = yes;ENTER = no>

76      Request #:EAL9793
77      You have selected the following options:
78          Convert N to NH4
79          Analysis Name      : NH4
80          Preparation Procedure # : N1347
81          Analytical Procedure # : EAL-fis-166
82          Hit ENTER if OK; any number or letter to change :
83          Detection limit (NH4) = 0.02571   Calcd: 0.025714
84          Original result : 0.073
85          880420-016 13164 NH4           C      5
86          0.094      UG/ML    N1347     EAL-fis-166
87          Calcd: 0.09386
88          Detection limit (NH4) = 0.02571
89          Original result : 0.072
90          880420-017 13164 NH4           C      6
91          0.093      UG/ML    N1347     EAL-fis-166
92          Detection limit (NH4) = 0.02571
93          Original result : 0.048
94          880420-018 13164 NH4           C      7
94          0.062      UG/ML    N1347     EAL-fis-166

```

95 Detection limit (NH4) = 0.02571
 96 Original result : 0.050
 97 880420-019 13164 NH4
 98 0.064 UG/ML N1347 C EAL-fis-166

99 Detection limit (NH4) = 0.02571
 100 Original result : 0.064
 101 880420-020 13164 NH4
 102 0.082 UG/ML N1347 C EAL-fis-166

103 Detection limit (NH4) = 0.02571
 104 Original result : 0.059
 105 880420-021 13164 NH4
 106 0.076 UG/ML N1347 C EAL-fis-166

107 Detection limit (NH4) = 0.02571
 108 Original result : 0.047
 109 880420-022 13164 NH4
 110 0.060 UG/ML N1347 C EAL-fis-166

111 Detection limit (NH4) = 0.02571
 112 Original result : 0.054
 113 880420-023 13164 NH4
 114 0.069 UG/ML N1347 C EAL-fis-166

115 Detection limit (NH4) = 0.02571
 116 Original result : 0.073
 117 880420-024 13164 NH4
 118 0.094 UG/ML N1347 C EAL-fis-166

119 Detection limit (NH4) = 0.02571
 120 Original result : 0.102
 121 880420-025 13164 NH4
 122 0.131 UG/ML N1347 C EAL-fis-166

123 Detection limit (NH4) = 0.02571
 124 Original result : 0.049
 125 880420-026 13164 NH4
 126 0.063 UG/ML N1347 C EAL-fis-166

127 Detection limit (NH4) = 0.02571 Calcd: 0.02571/
 128 Original result : 0.015
 129 880420-027 13164 NH4
 130 < 0.026 ✓ UG/ML N1347 C EAL-fis-166
 0.02571 ✓

131 Detection limit (NH4) = 0.02571
 132 Original result : 0.018
 133 880420-028 13164 NH4
 134 < 0.026 UG/ML N1347 C EAL-fis-166

135 Detection limit (NH4) = 0.02571
 136 Original result : 0.039
 137 880420-029 13164 NH4
 138 0.050 UG/ML N1347 C EAL-fis-166

139 Detection limit (NH4) = 0.02571
 140 Original result : 0.058
 141 880420-030 13164 NH4
 142 0.075 UG/ML N1347 C EAL-fis-166

143 Detection limit (NH4) = 0.02571
 144 Original result : 0.027
 145 880420-031 13164 NH4
 146 0.035 UG/ML N1347 C EAL-fis-166

147 Detection limit (NH4) = 0.02571
148 Original result : 0.039
149 880420-032 13164 NH4 C 21
150 0.050 UG/ML N1347 EAL-fis-166

151 Detection limit (NH4) = 0.02571
152 Original result : 0.041
153 880420-033 13164 NH4 C 22
154 0.053 UG/ML N1347 EAL-fis-166

155 Detection limit (NH4) = 0.02571
156 Original result : 0.066
157 880420-034 13164 NH4 C 23
158 0.085 UG/ML N1347 EAL-fis-166

159 Detection limit (NH4) = 0.02571
160 Original result : 0.029
161 880420-035 13164 NH4 C 24
162 0.037 UG/ML N1347 EAL-fis-166

163 Detection limit (NH4) = 0.02571
164 Original result : 0.038
165 880420-036 13164 NH4 C 25
166 0.049 UG/ML N1347 EAL-fis-166

167 Detection limit (NH4) = 0.02571
168 Original result : 0.022
169 880420-037 13164 NH4 C 26
170 0.028 UG/ML N1347 EAL-fis-166

171 Detection limit (NH4) = 0.02571
172 Original result : 0.047
173 880420-038 13164 NH4 C 27
174 0.060 UG/ML N1347 EAL-fis-166

175 :standard & result : 0.400 0.396

176 TKN/TKP 5/10/88 : analysis performed on FIS 880510 1515
177 Sequence # (ref): 8805100H

178 Request Numbers:
179 EAL9517 EAL9626
180 Total requests = 2
181 New tray-- hit ENTER to continue, or '\$' to skip tray

182 Select analytes to report:
183 1 - TKP
184 2 - TKN
185 Hit ENTER to report all analytes, or
186 enter the NUMBER(s) of the analyte(s) you want to report.

187 Enter '\$' if you want to process data by request #
188 Hit ENTER to process all requests

189 Is it OK to proceed?

190 Hit ENTER if OK; anything else to change

191	Cup #	1 s 0.100	0.090	0.098	1.00
192	Cup #	2 s 0.200	0.193 A-	0.199	1.00
193	Cup #	3 H2O	0.004	< x.xx D-	1.00
194	Cup #	4 EPA284-4	31.560	166.310 A-	500.00
195	Cup #	5 EPA	30.770	165.149 A-	500.00
196	Cup #	6 880216-297	0.301	0.873	4.00
197	Cup #	7 298	0.281	1.114 A-	4.00
198	Cup #	8 299	0.433	1.862 A-	4.00
199	Cup #	9 300	0.096	0.349	4.00
200	Cup #	10 301	0.164	0.311	4.00
201	Cup #	11 302	0.133	0.298	4.00
202	Cup #	12 303	0.073	0.194	4.00
203	Cup #	13 304	0.097	0.306	4.00
204	Cup #	14 305	0.079	0.192	4.00
205	Cup #	15 307	0.109	0.228	4.00
206	Cup #	16 308	0.079	0.191	4.00
207	Cup #	17 309	0.063	0.117	4.00
208	Cup #	18 BLK	0.016	< x.xx D-	1.00
209	i_blank_found =	1			
210	TKP		blank: 0.016		
211	TKN		blank: 0000.000		
212	Cup #	19 s 20ng	19.152 A-	19.953	100.00
213	Cup #	20 s 40ng	36.577	38.389 A-	100.00
214	Cup #	21 EPA486-2	130.895	HIGH A-	400.00
215	Cup #	22 880310-23	0.065	0.115	4.00
216	Cup #	23 24	0.074	0.375	4.00
217	Cup #	24 25-1	0.072	0.273	4.00
218	Cup #	25 25-2	0.086	0.280	4.00
219	Cup #	26 s 0.400	0.400	0.404 A-	1.00
220	Cup #	27 blk	0.014	< x.xx	
221	i_blank_found =	2			
222	TKP		blank: 0.014		
223	TKN		blank: 0000.000		
224	Cup #	28 blk	< x.xx	0.002	
225	i_blank_found =	3			
226	TKP		blank: 0000.000		
227	TKN		blank: 0.000		

228 There is more than one reagent blank.

229 To select blank result to use,
230 enter A, M(ean), N(ew) or D(elete).

231	A- Values for TKP	:
232	1 0.016	
233	2 0.014	
234	3 0.000	
235	Mean blank is	: 0.010
236	d	
237	Please enter the NUMBER of the blank to delete:	
238	3	
239	To select blank result to use,	
240	enter A, M(ean), N(ew) or D(elete).	

241	A- Values for Tkp	:
242	1 0.016	
243	2 0.014	
244	3 0.000	
245	Mean blank is	: 0.015
246	m	

247 To select blank result to use,
 248 enter A, M(ean), N(ew) or D(elete).
 249 A- Values for TKN :
 250 1 0.000
 251 2 0.000
 252 3 0.002
 253 Mean blank is : 0.001
 254 m
 255 Enter detection limit for TKP method.
 256 .001
 257 :standard & result : 0.100 0.090
 258 :standard & result : 0.200 0.193
 259 :water blank & result : 0.004
 260 EPA standard
 261 EPA standard
 262 SELECT OPTIONS -- Request # : EAL9517 See line 179
 263 Enter customer value for detection limit;otherwise,ENTER.
 264 Do you want to eliminate any results?<y=yes,ENTER=no>
 265 Enter 'P' to convert to another species :p
 266 Enter the NUMBER of the conversion to make:
 267 0--> P (no change)
 268 1--> PO4
 269 2--> H3PO4
 270 3--> P2O3
 271 4--> P2O4
 272 5--> P2O5
 273 2 Report phosphate as [H3PO4 = default] :
 274 Change Procedure #' ? <y = yes;ENTER = no>y
 276 Request #:EAL9517
 277 You have selected the following options:
 278 Convert P to : H3PO4
 279 Analysis Name : H3PO4
 280 Preparation Procedure # : To be changed
 281 Analytical Procedure # : To be changed
 282 Enter 'c' to subtract reagent blank;
 283 ENTER = no blank correction
 284 c
 285 Hit ENTER if OK; any number or letter to change :
 286 Enter preparation procedure # : P-9676
 287 Enter analysis procedure # : EAL-fis-2368 Calcd : 0.003/6
 288 Detection limit = 0.003
 289 Original result : 0.301
 290 880216-297 13164 H3PO4 C-B 6
 291 0.905 UG/ML P-9676 EAL-fis-2368
 292 (.301 - 0.015) X 3.16396 = 0.90482
 293 Detection limit = 0.003
 294 Original result : 0.281
 295 880216-298 13164 H3PO4 C-B 7
 296 0.842 UG/ML P-9676 EAL-fis-2368
 297 Detection limit = 0.003
 298 Original result : 0.433

298	880216-299	13164	H3PO4		C-B	8
299	1.323		UG/ML	P-9676	EAL-fis-2368	
300	Detection limit =	0.003				
301	Original result :	0.096				
302	880216-300	13164	H3PO4		C-B	9
303	0.256		UG/ML	P-9676	EAL-fis-2368	
304	Detection limit =	0.003				
305	Original result :	0.164				
306	880216-301	13164	H3PO4		C-B	10
307	0.471		UG/ML	P-9676	EAL-fis-2368	
308	Detection limit =	0.003				
309	Original result :	0.133				
310	880216-302	13164	H3PO4		C-B	11
311	0.373		UG/ML	P-9676	EAL-fis-2368	
312	Detection limit =	0.003				
313	Original result :	0.073				
314	880216-303	13164	H3PO4		C-B	12
315	0.184		UG/ML	P-9676	EAL-fis-2368	
316	Detection limit =	0.003				
317	Original result :	0.097				
318	880216-304	13164	H3PO4		C-B	13
319	0.259		UG/ML	P-9676	EAL-fis-2368	
320	Detection limit =	0.003				
321	Original result :	0.079				
322	880216-305	13164	H3PO4		C-B	14
323	0.202		UG/ML	P-9676	EAL-fis-2368	
324	Detection limit =	0.003				
325	Original result :	0.109				
326	880216-307	13164	H3PO4		C-B	15
327	0.297		UG/ML	P-9676	EAL-fis-2368	
328	Detection limit =	0.003				
329	Original result :	0.079				
330	880216-308	13164	H3PO4		C-B	16
331	0.202		UG/ML	P-9676	EAL-fis-2368	
332	Detection limit =	0.003				
333	Original result :	0.063				
334	880216-309	13164	H3PO4		C-B	17
335	0.152		UG/ML	P-9676	EAL-fis-2368	
336	:reagent blank & result :	0.016				
337	:standard & result :	20ng	19.152			
338	:standard & result :	40ng	36.577			
339	EPA standard					
340	SELECT OPTIONS -- Request # : EAL9626					
341	Enter customer value for detection limit;otherwise,ENTER.					
342	Do you want to eliminate any results?<y=yes,ENTER=no>					
343	Enter 'P' to convert to another species :					
344	Report phosphate as [P = default] :					
345	Change Procedure #' ? <y = yes;ENTER = no>					

```

346 Request #:EAL9626
347 You have selected the following options:
348 Analysis Name : P
349 Preparation Procedure # : P-9676
350 Analytical Procedure # : EAL-fis-2368
351 Enter 'c' to subtract reagent blank;
352 ENTER = no blank correction
353 c
354 Hit ENTER if OK; any number or letter to change :
355 Original result : 0.065
356 880310-023 13164 P *-B 22
357 0.050 UG/ML P-9676 EAL-fis-2368

$$0.065 - 0.015 = 0.050$$

358 Original result : 0.074
359 880310-024 13164 P *-B 23
360 0.059 UG/ML P-9676 EAL-fis-2368

361 Sub-sample # in error;now,25-1 25-1

362 Enter correct sub_sample # or
363 's' to skip result or 'd' to delete sample:
364 025
365 Original result : 0.072
366 880310-025 13164 P *-B 24
367 0.057 UG/ML P-9676 EAL-fis-2368

368 Sub-sample # in error;now,25-2 25-2

369 Enter correct sub_sample # or
370 's' to skip result or 'd' to delete sample:
371 025
372 Original result : 0.086
373 880310-025 13164 P *-B 25
374 0.071 UG/ML P-9676 EAL-fis-2368

375 :standard & result : 0.400 0.400
376 :reagent blank & result : 0.014
377 :reagent blank & result : < x.xx

378 Enter detection limit for TKN method.
379 .001
380 :standard & result : 0.100 0.098
381 :standard & result : 0.200 0.199
382 :water blank & result : < x.xx
383 EPA standard
384 EPA standard

385 SELECT OPTIONS -- Request # : EAL9517
386 Enter customer value for detection limit;otherwise,ENTER.
387 Do you want to eliminate any results?<y=yes,ENTER=no>

388 Enter 'N' to convert to 'NO3' :
389 Report nitrate as [N      = default] :

390 Change Procedure #'s ? <y = yes;ENTER = no>y

391 Request #:EAL9517
392 You have selected the following options:
393 Analysis Name : N
394 Preparation Procedure # : To be changed
395 Analytical Procedure # : To be changed

```

396 Enter 'c' to subtract reagent blank;
 397 ENTER = no blank correction
 398 c
 399 Hit ENTER if OK; any number or letter to change :
 400 Enter preparation procedure # : P-9676-N
 401 Enter analysis procedure # : EAL-fis-2346n
 402 Original result : 0.873
 403 880216-297 13164 N *-B 6
 404 0.872 UG/ML P-9676-N EAL-fis-2346n
 405 0.873 - 0.00 / = 0.872
 406 Original result : 1.114
 407 880216-298 13164 N *-B 7
 408 1.113 UG/ML P-9676-N EAL-fis-2346n
 409 Original result : 1.862
 410 880216-299 13164 N *-B 8
 411 1.861 UG/ML P-9676-N EAL-fis-2346n
 412 Original result : 0.349
 413 880216-300 13164 N *-B 9
 414 0.348 UG/ML P-9676-N EAL-fis-2346n
 415 Original result : 0.311
 416 880216-301 13164 N *-B 10
 417 0.310 UG/ML P-9676-N EAL-fis-2346n
 418 Original result : 0.298
 419 880216-302 13164 N *-B 11
 420 0.297 UG/ML P-9676-N EAL-fis-2346n
 421 Original result : 0.194
 422 880216-303 13164 N *-B 12
 423 0.193 UG/ML P-9676-N EAL-fis-2346n
 424 Original result : 0.306
 425 880216-304 13164 N *-B 13
 426 0.305 UG/ML P-9676-N EAL-fis-2346n
 427 Original result : 0.192
 428 880216-305 13164 N *-B 14
 429 0.191 UG/ML P-9676-N EAL-fis-2346n
 430 Original result : 0.228
 431 880216-307 13164 N *-B 15
 432 0.227 UG/ML P-9676-N EAL-fis-2346n
 433 Original result : 0.191
 434 880216-308 13164 N *-B 16
 435 0.190 UG/ML P-9676-N EAL-fis-2346n
 436 Original result : 0.117
 437 880216-309 13164 N *-B 17
 438 0.116 UG/ML P-9676-N EAL-fis-2346n
 439 :reagent blank & result : < x.xx
 440 :standard & result : 20ng 19.953
 441 :standard & result : 40ng 38.389
 EPA standard
 442 SELECT OPTIONS -- Request # : EAL9626
 443 Enter customer value for detection limit;otherwise,ENTER.

444 Do you want to eliminate any results? <y=yes,ENTER=no>
 445 Enter 'N' to convert to 'NO3' :
 446 Report nitrate as [N = default] :
 447 Change Procedure #'s ? <y = yes;ENTER = no>
 448 Request #:EAL9626
 449 You have selected the following options:
 450 Analysis Name : N
 451 Preparation Procedure # : P-9676-N
 452 Analytical Procedure # : EAL-fis-2346n
 453 Enter 'c' to subtract reagent blank;
 454 ENTER = no blank correction
 455 c
 456 Hit ENTER if OK; any number or letter to change :
 457 Original result : 0.115
 458 880310-023 13164 N *-B 22
 459 0.114 UG/ML P-9676-N EAL-fis-2346n

$$0.115 - 0.001 = 0.114$$

 460 Original result : 0.375
 461 880310-024 13164 N *-B 23
 462 0.374 UG/ML P-9676-N EAL-fis-2346n
 463 Original result : 0.273
 464 880310-025 13164 N *-B 24 Sample #
 465 0.272 UG/ML P-9676-N EAL-fis-2346n corrected
 466 Original result : 0.280
 467 880310-025 13164 N *-B 25
 468 0.279 UG/ML P-9676-N EAL-fis-2346n
 469 :standard & result : 0.400 0.404
 470 :reagent blank & result : < x.xx
 471 :reagent blank & result : 0.002
 472 NH3 salicylate : analysis performed on FIS 880511 1533
 473 Sequence # (ref): 8805110H
 474 Request Numbers:
 475 EAL9793 EAL9751 EAL9752
 476 Total requests = 3
 477 New tray-- hit ENTER to continue, or '\$' to skip tray
 478 Enter '\$' if you want to process data by request #
 479 Hit ENTER to process all requests
 480 \$
 481 OPTION: S(ave) or D(elete) ?
 482 If you (S)ave one or more requests, only those 'saved'
 will be processed.
 483 If you (D)elete one or more requests, those not deleted
 will be processed.

486 Valid requests :
 487 EAL9793 EAL9751 EAL9752
 488 Please enter S or D
 489 d
 490 Enter the request #(s) to delete:
 491 EXAMPLE: 9996;9975;...;9966(no spaces,do not enter EAL)
 492 Hit ENTER to process all requests.
 493 9751

494 Number of requests to delete: = 1

495 EAL9751 will not be processed
 496 Is it OK to proceed?

497 Hit ENTER if OK; anything else to change

498 Cup #	1 H2O	0.006	1.00
499 Cup #	2 s 0.050	0.042	1.00
500 Cup #	3 s 0.100	0.100	1.00
501 Cup #	4 Pet-3	55.001 A-	100.00
502 Cup #	5 Pet-4	156.999 A-	262.50
503 Cup #	6 pet-1	25.067	200.00
504 Cup #	7 Pet-2	210.689 A-	500.00
505 Cup #	8 880420-56	0.019	1.00
506 Cup #	9 57	0.017	1.00
507 Cup #	10 58	0.020	1.00
508 Cup #	11 59	0.020	1.00
509 Cup #	12 60	0.022	1.00
510 Cup #	13 61	0.029	1.00
511 Cup #	14 62	0.046	1.00
512 Cup #	15 63	0.048	1.00
513 Cup #	16 64	0.020	1.00
514 Cup #	17 880411-38	0.004	1.00
515 Cup #	18 QNS 39	0.003	1.00
516 Cup #	19 40	0.010	1.00
517 Cup #	20 880411-41	0.116	1.00
518 Cup #	21 42	0.618 A-	1.00
519 Cup #	22 43	0.186	1.00
520 Cup #	23 44	0.089	1.00
521 Cup #	24 45	0.202	1.00
522 Cup #	25 46	0.137	1.00
523 Cup #	26 47	0.017	1.00
524 Cup #	27 48	0.495 A-	1.00
525 Cup #	28 49	0.025	1.00
526 Cup #	29 50	0.354 A-	1.00
527 Cup #	30 51	0.540 A-	1.00
528 Cup #	31 s 0.400	0.407 A-	1.00

See line 493
EAL9751

529 Enter detection limit for NH3/N method.
 530 .001
 531 :water blank & result : 0.006
 532 :standard & result : 0.050 0.042
 533 :standard & result : 0.100 0.100
 534 Pet sample
 535 Pet sample
 536 Pet sample
 537 Pet sample

538 SELECT OPTIONS -- Request # : EAL9793
 539 Enter customer value for detection limit;otherwise,ENTER.
 540 .02
 541 Do you want to eliminate any results?<y=yes,ENTER=no>

542 Enter '3' to convert 'N' to 'NH3' :
 543 Enter '4' to convert 'N' to 'NH4' :
 544 Report ammonia as [N = default] :
 545 Change Procedure #'s ? <y = yes;ENTER = no>y
 546 Request #:EAL9793
 547 You have selected the following options:
 548 NH3 to be reported as N
 549 Analysis Name : N
 550 Preparation Procedure # : To be changed
 551 Analytical Procedure # : To be changed
 552 Hit ENTER if OK; any number or letter to change :
 553 Enter preparation procedure # : N-123
 554 Enter analysis procedure # : EAL-fis-9763
 555 880420-056 13164 N * 8
 556 < 0.020 UG/ML N-123 EAL-fis-9763
 557 880420-057 13164 N * 9
 558 < 0.020 UG/ML N-123 EAL-fis-9763
 559 880420-058 13164 N * 10
 560 0.020 UG/ML N-123 EAL-fis-9763
 561 880420-059 13164 N * 11
 562 0.020 UG/ML N-123 EAL-fis-9763
 563 880420-060 13164 N * 12
 564 0.022 UG/ML N-123 EAL-fis-9763
 565 880420-061 13164 N * 13
 566 0.029 UG/ML N-123 EAL-fis-9763
 567 880420-062 13164 N * 14
 568 0.046 UG/ML N-123 EAL-fis-9763
 569 880420-063 13164 N * 15
 570 0.048 UG/ML N-123 EAL-fis-9763
 571 880420-064 13164 N * 16
 572 0.020 UG/ML N-123 EAL-fis-9763
 573 special material & results :QNS 39 0.003 1.00
 574 SELECT OPTIONS -- Request # : EAL9752
 575 Enter customer value for detection limit;otherwise,ENTER.
 576 Do you want to eliminate any results?<y=yes,ENTER=no>
 577 Enter '3' to convert 'N' to 'NH3' :
 578 Enter '4' to convert 'N' to 'NH4' :
 579 Report ammonia as [N = default] :
 580 Change Procedure #'s ? <y = yes;ENTER = no>
 581 Request #:EAL9752
 582 You have selected the following options:
 583 NH3 to be reported as N
 584 Analysis Name : N
 585 Preparation Procedure # : N-123

Vials 17 & 19
 not reported -
 correct!
 See line 493

586 Analytical Procedure # : EAL-fis-9763
 587 Hit ENTER if OK; any number or letter to change :
 588 880411-041 13164 N • 20
 589 0.116 UG/ML N-123 EAL-fis-9763
 590 880411-042 13164 N • 21
 591 0.618 UG/ML N-123 EAL-fis-9763
 592 880411-043 13164 N * 22
 593 0.186 UG/ML N-123 EAL-fis-9763
 594 880411-044 13164 N * 23
 595 0.089 UG/ML N-123 EAL-fis-9763
 596 880411-045 13164 N • 24
 597 0.202 UG/ML N-123 EAL-fis-9763
 598 880411-046 13164 N * 25
 599 0.137 UG/ML N-123 EAL-fis-9763
 600 880411-047 13164 N • 26
 601 0.017 UG/ML N-123 EAL-fis-9763
 602 880411-048 13164 N • 27
 603 0.495 UG/ML N-123 EAL-fis-9763
 604 880411-049 13164 N • 28
 605 0.025 UG/ML N-123 EAL-fis-9763
 606 880411-050 13164 N * 29
 607 0.354 UG/ML N-123 EAL-fis-9763
 608 880411-051 13164 N * 30
 609 0.540 UG/ML N-123 EAL-fis-9763
 610 :standard & result : 0.400 0.407

611 TKN/TKP 5/10/88 : analysis performed on FIS 880511 1008
 612 Sequence # (ref): 8805110C

613 Request Numbers:
 614 EAL9626
 615 Total requests = 1
 616 New tray-- hit ENTER to continue,or '\$' to skip tray
 617 Select analytes to report:
 618 1 - TKP
 619 2 - TKN
 620 Hit ENTER to report all analytes, or
 621 enter the NUMBER(s) of the analyte(s) you want to report.
 622 Is it OK to proceed?
 623 Hit ENTER if OK; anything else to change
 624 g
 625 New tray-- hit ENTER to continue,or '\$' to skip tray
 626 Select analytes to report:
 627 1 - TKP
 628 2 - TKN
 629 Hit ENTER to report all analytes, or
 630 enter the NUMBER(s) of the analyte(s) you want to report.

631 1
 632 Enter next number; terminate list with ENTER only
 633 Is it OK to proceed?
 634 Hit ENTER if OK; anything else to change
 635 Cup # 1 H2O 0.018 < x.xx D- 1.00
 636 Cup # 2 s 0.100 0.093 0.099 1.00
 637 Cup # 3 s 0.200 0.190 A- 0.197 1.00
 638 Cup # 4 s 0.400 0.401 0.403 A- 1.00
 639 Cup # 5 EPA284-4 29.780 165.500 A- 500.00
 640 Cup # 6 EPA 30.884 166.363 A- 500.00
 641 Cup # 7 880310-26-1 0.143 0.335 4.00 - Note incorrect
 642 Cup # 8 26-2 0.092 0.295 4.00
 643 Cup # 9 27 0.100 0.295 4.00
 644 Cup # 10 28 0.126 0.336 4.00
 645 Cup # 11 29 0.102 0.271 4.00
 646 Cup # 12 30 0.120 0.239 4.00
 647 Cup # 13 31 0.091 0.171 4.00
 648 Cup # 14 32 0.076 0.164 4.00
 649 Cup # 15 33 0.084 0.255 4.00
 650 Cup # 16 34 0.080 0.203 4.00
 651 Cup # 17 35 0.083 0.227 4.00
 652 Cup # 18 36 0.089 0.181 4.00
 653 Cup # 19 37 0.123 0.182 4.00
 654 Cup # 20 38 0.110 0.232 4.00
 655 Cup # 21 s 0.200 0.188 A- 0.194 1.00
 656 Cup # 22 39 0.091 0.240 4.00
 657 Cup # 23 40 0.147 0.148 4.00
 658 Cup # 24 41 0.068 0.269 4.00
 659 Cup # 25 BLK 0.025 < x.xx D- 1.00
 660 i_blank_found = 1
 661 TKP blank: 0.025
 662 TKN blank: 0000.000
 663 Cup # 26 s 40ng 36.103 38.784 A- 100.00
 664 Cup # 27 EPA486-2 130.720 497.250 A- 1050.00
 665 Cup # 28 43 0.142 0.490 4.00
 666 Cup # 29 47 0.128 0.750 4.00
 667 Cup # 30 s 0.400 0.401 0.402 A- 1.00

668 Enter detection limit for TKP method.
 669 .001
 670 :water blank & result : 0.018
 671 :standard & result : 0.100 0.093
 672 :standard & result : 0.200 0.190
 673 :standard & result : 0.400 0.401
 674 EPA standard
 675 EPA standard
 676 Sub-sample # in error; now, 880310-26-1 - Incorrect sample #
 677 Enter correct sub_sample # or
 678 's' to skip result or 'd' to delete sample:
 679 026
 680 SELECT OPTIONS -- Request # : EAL9626
 681 Enter customer value for detection limit; otherwise, ENTER.
 682 Do you want to eliminate any results? <y=yes,ENTER=no>
 683 Enter 'P' to convert to another species :
 684 Report phosphate as [P = default] :
 685 Change Procedure #' ? <y = yes;ENTER = no>

Sample #
(See line 676)

Incorrect sample #
trapped.

686 Request #:EAL9626
 687 You have selected the following options:
 688 Analysis Name : P
 689 Preparation Procedure # :
 690 Analytical Procedure # :
 691 Enter 'c' to subtract reagent blank;
 692 ENTER = no blank correction
 693
 694 Hit ENTER if OK; any number or letter to change :
 695 There is no preparation procedure #
 696 Enter #, or hit ENTER to leave blank:
 697 There is no analysis procedure
 698 Enter #, or hit ENTER to leave blank:
 699 Original result : 0.143
 700 880310-026 13164 P *-B
 701 0.118 UG/ML
 702 Sub-sample # in error; now, 26-2 26-2
 703 Enter correct sub_sample # or
 704 's' to skip result or 'd' to delete sample:
 705
026
 706 Original result : 0.092
 707 880310-026 13164 P *-B
 708 0.067 UG/ML
 709 Original result : 0.100
 710 880310-027 13164 P *-B
 711 0.075 UG/ML
 712 Original result : 0.126
 713 880310-028 13164 P *-B
 714 0.101 UG/ML
 715 Original result : 0.102
 716 880310-029 13164 P *-B
 717 0.077 UG/ML
 718 Original result : 0.120
 719 880310-030 13164 P *-B
 720 0.095 UG/ML
 721 Original result : 0.091
 722 880310-031 13164 P *-B
 723 0.066 UG/ML
 724 Original result : 0.076
 725 880310-032 13164 P *-B
 726 0.051 UG/ML
 727 Original result : 0.084
 728 880310-033 13164 P *-B
 729 0.059 UG/ML
 730 Original result : 0.080
 731 880310-034 13164 P *-B
 732 0.055 UG/ML
 733 Original result : 0.083
 734 880310-035 13164 P *-B
 735 0.058 UG/ML

0.143
 7 -0.025
0.118

8 Note corrected
 sample #
 0.092
 9 -0.025
0.067 (vial 8)

736 Original result : 0.089
 737 880310-036 13164 P *-B 18
 738 0.064 UG/ML

739 Original result : 0.123
 740 880310-037 13164 P *-B 19
 741 0.098 UG/ML

742 Original result : 0.110
 743 880310-038 13164 P *-B 20
 744 0.085 UG/ML

745 :standard & result : 0.200 0.188
 746 Original result : 0.091
 747 880310-039 13164 P *-B 22
 748 0.066 UG/ML

749 Original result : 0.147
 750 880310-040 13164 P *-B 23
 751 0.122 UG/ML

752 Original result : 0.068
 753 880310-041 13164 P *-B 24
 754 0.043 UG/ML

755 :reagent blank & result : 0.025
 756 :standard & result : 40ng 36.103
 757 EPA standard

758 Original result : 0.142
 759 880310-043 13164 P *-B 28
 760 0.117 UG/ML

761 Original result : 0.128
 762 880310-047 13164 P *-B 29
 763 0.103 UG/ML

764 :standard & result : 0.400 0.401 Program does not
 process TKN - line 631

765 TKN/TKP 5/10/88 : analysis performed on FIS 880511 1216
 766 Sequence # (ref): 8805110D

767 Request Numbers:
 768 EAL9626

769 Total requests = 1
 770 New tray-- hit ENTER to continue, or '\$' to skip tray

771 \$

772 TKN/TKP 5/10/88 : analysis performed on FIS 880511 1314
 773 Sequence # (ref): 8805110E

774 Request Numbers:
 775 EAL9626

776 Total requests = 1
 777 New tray-- hit ENTER to continue, or '\$' to skip tray

778 \$

779 NH3 salicylate : analysis performed on FIS 880511 1444
 780 Sequence # (ref): 8805110G

781 Request Numbers:
 782 EAL9793
 783 Total requests = 1
 784 New tray-- hit ENTER to continue,or '\$' to skip tray

785 Is it OK to proceed?

786 Hit ENTER if OK; anything else to change

787 Cup #	1 H2O	0.002	1.00
788 Cup #	2 s 0.050	0.046	1.00
789 Cup #	3 s 0.100	0.101	1.00
790 Cup #	4 Pet-3	HIGH A-	100.00
791 Cup #	5 Pet-4	156.545 A-	262.50
792 Cup #	6 Pet-1	26.789	200.00
793 Cup #	7 Pet-2	213.605 A-	500.00
794 Cup #	8 H2O	< x.xx D-	1.00
795 Cup #	9 880420-37	0.018	1.00
796 Cup #	10 38	0.044	1.00
797 Cup #	11 39	0.037	1.00
798 Cup #	12 40	0.059	1.00
799 Cup #	13 41	0.078	1.00
800 Cup #	14 42	0.045	1.00
801 Cup #	15 43	0.053	1.00
802 Cup #	16 44	0.092	1.00
803 Cup #	17 45	0.044	1.00
804 Cup #	18 46	0.079	1.00
805 Cup #	19 47	0.106	1.00
806 Cup #	20 48	0.043	1.00
807 Cup #	21 49	0.033	1.00
808 Cup #	22 50	0.039	1.00
809 Cup #	23 51	0.084	1.00
810 Cup #	24 52	0.008	1.00
811 Cup #	25 53	0.022	1.00
812 Cup #	26 54	0.025	1.00
813 Cup #	27 55	0.018	1.00
814 Cup #	28 s0.400	0.407 A-	1.00

815 Enter detection limit for NH3/N method.

.001

817 :water blank & result : 0.002
 818 :standard & result : 0.050 0.046
 819 :standard & result : 0.100 0.101
 820 Pet sample
 821 Pet sample
 822 Pet sample
 823 Pet sample
 824 :water blank & result : < x.xx

825 SELECT OPTIONS -- Request # : EAL9793

826 Enter customer value for detection limit;otherwise,ENTER.

.05

828 Do you want to eliminate any results?<y=yes,ENTER=no>

829 Enter '3' to convert 'N' to 'NH3' :

830 Enter '4' to convert 'N' to 'NH4' : 4

831 Report ammonia as [NH4 = default] :

832 ammonia as phosphate

833 Change Procedure #'s ? <y = yes;ENTER = no>

- operator error mode

834 Request #:EAL9793
 835 You have selected the following options:
 836 Convert N to NH4
 837 Analysis Name : ammonia as phosphate
 838 Preparation Procedure # :
 839 Analytical Procedure # :
 840 Hit ENTER if OK; any number or letter to change : w *Correction requested*

 841 SELECT OPTIONS -- Request # : EAL9793
 842 Enter customer value for detection limit;otherwise,ENTER.
.05
 844 Do you want to eliminate any results?<y=yes,ENTER=no>

 845 Enter '3' to convert 'N' to 'NH3' :
 846 Enter '4' to convert 'N' to 'NH4' : 4
 847 Report ammonia as [NH4 = default] :
 848 ammonia as ion
 849 Change Procedure #'s ? <y = yes;ENTER = no> *- Correction made*

 850 Request #:EAL9793
 851 You have selected the following options:
 852 Convert N to NH4
 853 Analysis Name : ammonia as ion
 854 Preparation Procedure # :
 855 Analytical Procedure # :
 856 Hit ENTER if OK; any number or letter to change :

 857 There is no preparation procedure #
 858 Enter #, or hit ENTER to leave blank:

 859 There is no analysis procedure
 860 Enter #, or hit ENTER to leave blank: *Calcd detection limit = 0.064286*

 861 Detection limit (NH4) = 0.06429
 862 Original result : 0.018
 863 880420-037 13164 ammonia as ion
 864 < 0.064 UG/ML *0.018 x 1.28571 = 0.023143 < 0.064*
Correct *C 9 Correct Name*
 865 Detection limit (NH4) = 0.06429
 866 Original result : 0.044
 867 880420-038 13164 ammonia as ion
 868 < 0.064 UG/ML C 10

 869 Detection limit (NH4) = 0.06429
 870 Original result : 0.037
 871 880420-039 13164 ammonia as ion
 872 < 0.064 UG/ML C 11

 873 Detection limit (NH4) = 0.06429
 874 Original result : 0.059
 875 880420-040 13164 ammonia as ion
 876 0.076 UG/ML C 12

 877 Detection limit (NH4) = 0.06429
 878 Original result : 0.078
 879 880420-041 13164 ammonia as ion
 880 0.100 UG/ML C 13

881	Detection limit (NH4) = 0.06429			
882	Original result : 0.045			
883	880420-042 13164 ammonia as ion	C	14	
884	< 0.064 UG/ML			
885	Detection limit (NH4) = 0.06429			
886	Original result : 0.053			
887	880420-043 13164 ammonia as ion	C	15	
888	0.068 UG/ML			
889	Detection limit (NH4) = 0.06429			
890	Original result : 0.092			
891	880420-044 13164 ammonia as ion	C	16	
892	0.118 UG/ML			
893	Detection limit (NH4) = 0.06429			
894	Original result : 0.044			
895	880420-045 13164 ammonia as ion	C	17	
896	< 0.064 UG/ML			
897	Detection limit (NH4) = 0.06429			
898	Original result : 0.079			
899	880420-046 13164 ammonia as ion	C	18	
900	0.102 UG/ML			
901	Detection limit (NH4) = 0.06429			
902	Original result : 0.106			
903	880420-047 13164 ammonia as ion	C	19	
904	0.136 UG/ML			
905	Detection limit (NH4) = 0.06429			
906	Original result : 0.043			
907	880420-048 13164 ammonia as ion	C	20	
908	< 0.064 UG/ML			
909	Detection limit (NH4) = 0.06429			
910	Original result : 0.033			
911	880420-049 13164 ammonia as ion	C	21	
912	< 0.064 UG/ML			
913	Detection limit (NH4) = 0.06429			
914	Original result : 0.039			
915	880420-050 13164 ammonia as ion	C	22	
916	< 0.064 UG/ML			
917	Detection limit (NH4) = 0.06429			
918	Original result : 0.084			
919	880420-051 13164 ammonia as ion	C	23	
920	0.108 UG/ML			
921	Detection limit (NH4) = 0.06429			
922	Original result : 0.008			
923	880420-052 13164 ammonia as ion	C	24	
924	< 0.064 UG/ML			
925	Detection limit (NH4) = 0.06429			
926	Original result : 0.022			
927	880420-053 13164 ammonia as ion	C	25	
928	< 0.064 UG/ML			
929	Detection limit (NH4) = 0.06429			
930	Original result : 0.025			
931	880420-054 13164 ammonia as ion	C	26	
932	< 0.064 UG/ML			

933 Detection limit (NH4) = 0.06429
 934 Original result : 0.018
 935 880420-055 13164 ammonia as ion C 27
 936 < 0.064 UG/ML

937 :standard & result : 0.400 0.407

938 NH3 salicylate : analysis performed on FIS 880512 0937
 939 Sequence # (ref): 8805120B

940 Request Numbers:
 941 EAL9753 EAL9754
 942 Total requests = 2
 943 New tray-- hit ENTER to continue, or '\$' to skip tray

944 \$

945 NH3 salicylate : analysis performed on FIS 880512 1521
 946 Sequence # (ref): 8805120H

947 Request Numbers:
 948 EAL9785 EAL9786
 949 Total requests = 2
 950 New tray-- hit ENTER to continue, or '\$' to skip tray

951 Enter '\$' if you want to process data by request #
 952 Hit ENTER to process all requests

953 Is it OK to proceed?

954 Hit ENTER if OK; anything else to change

955	Cup #	1 H2O	0.008	1.00
956	Cup #	2 s 0.050	0.056	1.00
957	Cup #	3 s 0.100	0.118	1.00
958	Cup #	4 880419-55	0.083	1.00
959	Cup #	5 56	0.087	1.00
960	Cup #	6 57	0.104	1.00
961	Cup #	7 58	0.140	1.00
962	Cup #	8 59	0.162	1.00
963	Cup #	9 60	0.040	1.00
964	Cup #	10 61	0.172	1.00
965	Cup #	11 62	0.165	1.00
966	Cup #	12 63	0.231	1.00
967	Cup #	13 64	0.032	1.00
968	Cup #	14 880419-65	0.310 A-	1.00
969	Cup #	15 66	0.315 A-	1.00
970	Cup #	16 67	0.324 A-	1.00
971	Cup #	17 68	0.314 A-	1.00
972	Cup #	18 69	0.278 A-	1.00
973	Cup #	19 70	0.296 A-	1.00
974	Cup #	20 71	0.301 A-	1.00
975	Cup #	21 72	0.360 A-	1.00
976	Cup #	22 73	0.368 A-	1.00
977	Cup #	23 74	HIGH A-	1.00
978	Cup #	24 750NS	0.019	1.00
979	Cup #	25 76	0.012	1.00

```

980    Cup # 26 77      0.013      1.00
981    Cup # 27 78      0.012      1.00
982    Cup # 28 79      0.015      1.00
983    Cup # 29 84      0.092      1.00
984    Cup # 30 85      0.075      1.00
985    Cup # 31 s 0.400  0.419 A-   1.00

```

```

986    Enter detection limit for NH3/N method.
987    .001
988    :water blank & result : 0.008
989    :standard & result : 0.050  0.056
990    :standard & result : 0.100  0.118

991    SELECT OPTIONS -- Request # : EAL9785
992    Enter customer value for detection limit;otherwise,ENTER.

993    Do you want to eliminate any results?<y=yes,ENTER=no>

994    Enter '3' to convert 'N' to 'NH3' :
995    Enter '4' to convert 'N' to 'NH4' :
996    Report ammonia as [N = default] :

997    Change Procedure #'s ? <y = yes;ENTER = no>y

```

```

998    Request #:EAL9785
999    You have selected the following options:
1000    NH3 to be reported as N
1001    Analysis Name : N
1002    Preparation Procedure # : To be changed
1003    Analytical Procedure # : To be changed
1004    Hit ENTER if OK; any number or letter to change :

1005    Enter preparation procedure # : N-123
1006    Enter analysis procedure # : EAL-fis-6663

1007    880419-055 13164 N * 4
1008    0.083       UG/ML  N-123  EAL-fis-6663

1009    880419-056 13164 N * 5
1010    0.087       UG/ML  N-123  EAL-fis-6663

1011    880419-057 13164 N * 6
1012    0.104       UG/ML  N-123  EAL-fis-6663

1013    880419-058 13164 N * 7
1014    0.140       UG/ML  N-123  EAL-fis-6663

1015    880419-059 13164 N * 8
1016    0.162       UG/ML  N-123  EAL-fis-6663

1017    880419-060 13164 N * 9
1018    0.040       UG/ML  N-123  EAL-fis-6663

1019    880419-061 13164 N * 10
1020    0.172       UG/ML  N-123  EAL-fis-6663

1021    880419-062 13164 N * 11
1022    0.165       UG/ML  N-123  EAL-fis-6663

1023    880419-063 13164 N * 12
1024    0.231       UG/ML  N-123  EAL-fis-6663

```

1025 880419-064 13164 N * 13
 1026 0.032 UG/ML N-123 EAL-fis-6663

1027 SELECT OPTIONS -- Request # : EAL9786
 1028 Enter customer value for detection limit;otherwise,ENTER.

1029 Do you want to eliminate any results? <y=yes,ENTER=no>

1030 Enter '3' to convert 'N' to 'NH3' :
 1031 Enter '4' to convert 'N' to 'NH4' :
 1032 Report ammonia as [N = default] :

1033 Change Procedure #'s ? <y = yes;ENTER = no>

1034 Request #:EAL9786
 1035 You have selected the following options:
 1036 NH3 to be reported as N
 1037 Analysis Name : N
 1038 Preparation Procedure # : N-123
 1039 Analytical Procedure # : EAL-fis-6663
 1040 Hit ENTER if OK; any number or letter to change :

1041 880419-065 13164 N * 14
 1042 0.310 UG/ML N-123 EAL-fis-6663

1043 880419-066 13164 N * 15
 1044 0.315 UG/ML N-123 EAL-fis-6663

1045 880419-067 13164 N * 16
 1046 0.324 UG/ML N-123 EAL-fis-6663

1047 880419-068 13164 N * 17
 1048 0.314 UG/ML N-123 EAL-fis-6663

1049 880419-069 13164 N * 18
 1050 0.278 UG/ML N-123 EAL-fis-6663

1051 880419-070 13164 N * 19
 1052 0.296 UG/ML N-123 EAL-fis-6663

1053 880419-071 13164 N * 20
 1054 0.301 UG/ML N-123 EAL-fis-6663

1055 880419-072 13164 N * 21
 1056 0.360 UG/ML N-123 EAL-fis-6663

1057 880419-073 13164 N * 22
 1058 0.368 UG/ML N-123 EAL-fis-6663

1059 880419-074 23 074 HIGH A- 1.00
 1060 High result--no entry in Analis. Hit enter to continue

1061 880419-074 13164 N * 23 See line 977
 1062 > UG/ML N-123 EAL-fis-6663
 1063 Sub-sample # in error;now,75QNS 75QN

1064 Enter correct sub_sample # or
 1065 's' to skip result or 'd' to delete sample:

d 880419-076 13164 N * 25
 1067 0.012 UG/ML N-123 EAL-fis-6663

-#24 deleted

1069	880419-077	13164	N		*	26
1070	0.013		UG/ML	N-123	EAL-fis-6663	
1071	880419-078	13164	N		*	27
1072	0.012		UG/ML	N-123	EAL-fis-6663	
1073	880419-079	13164	N		*	28
1074	0.015		UG/ML	N-123	EAL-fis-6663	
1075	880419-084	13164	N		*	29
1076	0.092		UG/ML	N-123	EAL-fis-6663	
1077	880419-085	13164	N		*	30
1078	0.075		UG/ML	N-123	EAL-fis-6663	
1079	:standard & result :			0.400	0.419	
1080	Deleted :			24 x5QNS	0.019	1.00

1081 NH3 salicylate : analysis performed on FIS 880512 1023
 1082 Sequence # (ref): 8805120C

1083 Request Numbers:
 1084 EAL9754
 1085 Total requests = 1
 1086 New tray-- hit ENTER to continue, or '\$' to skip tray

1087 \$

1088 NH3 salicylate : analysis performed on FIS 880512 1238
 1089 Sequence # (ref): 8805120D

1090 Request Numbers:
 1091 EAL9755
 1092 Total requests = 1
 1093 New tray-- hit ENTER to continue, or '\$' to skip tray

1094 \$

1095 Total vials: 176 from 6 trays.
 1096 of these, 1 was high (not reported)

1097	Standards :	23
1098	W-Blanks :	7
1099	R-Blanks :	4
1100	EPA stds :	6
1101	Pet's :	8
1102	Other :	1

1103 Samples : 127 *Sum = 176 (gl. line 1095)*
 1104 < detect : 16
 1105 Deleted : 3 (includes high results)

1106 NH3/N 's deleted : 0
 1107 Prepared with fis_parse, version : 9/20/88 ✓
 1108 \$

THIS PAGE LEFT BLANK INTENTIONALLY

APPENDIX D
SAMPLE OF DATA AFTER FORMATTING BY FIS_PARSE

This appendix lists the data stored in FILE_TRANSFER.DAT by FIS_PARSE during processing for storage in AnaLis. Only the data to the right of the colons are in FILE_TRANSFER.DAT. The data are contiguous; i.e., there is no space between Anal Procedure and Sample # in the disc file (File_Transfer.dat). This Appendix does not present the entire file.

```
1      Readings taken from 'File transfer.dat'.
2      The same data are stored in file : temp01.dat
3      Hit ENTER when ready to proceed.

4      Sample #      : 880331-293
5      Operator badge #: 13164
6      Analysis name  : NH3
7      Limits exceeded :
8      Results       : 0.275
9      Error          :
10     Units          : UG/ML
11     Prep Procedure : N1347
12     Anal Procedure : EAL-fis-166
13
14     Sample #      : 880420-016
15     Operator badge #: 13164
16     Analysis name  : NH4
17     Limits exceeded :
18     Results       : 0.094
19     Error          :
20     Units          : UG/ML
21     Prep Procedure : N1347
22     Anal Procedure : EAL-fis-166
23
24     Sample #      : 880420-017
25     Operator badge #: 13164
26     Analysis name  : NH4
27     Limits exceeded :
28     Results       : 0.093
29     Error          :
30     Units          : UG/ML
31     Prep Procedure : N1347
32     Anal Procedure : EAL-fis-166
33
34     Sample #      : 880420-018
35     Operator badge #: 13164
36     Analysis name  : NH4
37     Limits exceeded :
38     Results       : 0.062
39     Error          :
40     Units          : UG/ML
41     Prep Procedure : N1347
42     Anal Procedure : EAL-fis-166
```

43 Sample # : 880420-037
44 Operator badge #: 13164
45 Analysis name : NH4
46 Limits exceeded :
47 Results : 0.028
48 Error :
49 Units : UG/ML
50 Prep Procedure : N1347
51 Anal Procedure : EAL-fis-166
52
53 Sample # : 880420-038
54 Operator badge #: 13164
55 Analysis name : NH4
56 Limits exceeded :
57 Results : 0.060
58 Error :
59 Units : UG/ML
60 Prep Procedure : N1347
61 Anal Procedure : EAL-fis-166
62
63 Sample # : 880216-297
64 Operator badge #: 13164
65 Analysis name : H3PO4
66 Limits exceeded :
67 Results : 0.905
68 Error :
69 Units : UG/ML
70 Prep Procedure : P-9676
71 Anal Procedure : EAL-fis-2368
72
73 Sample # : 880216-298
74 Operator badge #: 13164
75 Analysis name : H3PO4
76 Limits exceeded :
77 Results : 0.842
78 Error :
79 Units : UG/ML
80 Prep Procedure : P-9676
81 Anal Procedure : EAL-fis-2368
82
83 Sample # : 880216-304
84 Operator badge #: 13164
85 Analysis name : H3PO4
86 Limits exceeded :
87 Results : 0.259
88 Error :
89 Units : UG/ML
90 Prep Procedure : P-9676
91 Anal Procedure : EAL-fis-2368
92
93 Sample # : 880216-305

94 Operator badge #: 13164
95 Analysis name : H3PO4
96 Limits exceeded :
97 Results : 0.202
98 Error :
99 Units : UG/ML
100 Prep Procedure : P-9676
101 Anal Procedure : EAL-fis-2368
102
103 Sample # : 880216-307
104 Operator badge #: 13164
105 Analysis name : H3PO4
106 Limits exceeded :
107 Results : 0.297
108 Error :
109 Units : UG/ML
110 Prep Procedure : P-9676
111 Anal Procedure : EAL-fis-2368
112
113 Sample # : 880216-308
114 Operator badge #: 13164
115 Analysis name : H3PO4
116 Limits exceeded :
117 Results : 0.202
118 Error :
119 Units : UG/ML
120 Prep Procedure : P-9676
121 Anal Procedure : EAL-fis-2368
122
123 Sample # : 880216-309
124 Operator badge #: 13164
125 Analysis name : H3PO4
126 Limits exceeded :
127 Results : 0.152
128 Error :
129 Units : UG/ML
130 Prep Procedure : P-9676
131 Anal Procedure : EAL-fis-2368
132
133 Sample # : 880310-023
134 Operator badge #: 13164
135 Analysis name : P
136 Limits exceeded :
137 Results : 0.050
138 Error :
139 Units : UG/ML
140 Prep Procedure : P-9676
141 Anal Procedure : EAL-fis-2368
142
143 Sample # : 880310-024
144 Operator badge #: 13164

145 Analysis name : P
146 Limits exceeded :
147 Results : 0.059
148 Error :
149 Units : UG/ML
150 Prep Procedure : P-9676
151 Anal Procedure : EAL-fis-2368
152
153 Sample # : 880310-025
154 Operator badge # : 13164
155 Analysis name : P
156 Limits exceeded :
157 Results : 0.057
158 Error :
159 Units : UG/ML
160 Prep Procedure : P-9676
161 Anal Procedure : EAL-fis-2368
162
163 Sample # : 880310-025
164 Operator badge # : 13164
165 Analysis name : P
166 Limits exceeded :
167 Results : 0.071
168 Error :
169 Units : UG/ML
170 Prep Procedure : P-9676
171 Anal Procedure : EAL-fis-2368
172
173 Sample # : 880216-297
174 Operator badge # : 13164
175 Analysis name : N
176 Limits exceeded :
177 Results : 0.872
178 Error :
179 Units : UG/ML
180 Prep Procedure : P-9676-N
181 Anal Procedure : EAL-fis-2346n
182
183 Sample # : 880216-298
184 Operator badge # : 13164
185 Analysis name : N
186 Limits exceeded :
187 Results : 1.113
188 Error :
189 Units : UG/ML
190 Prep Procedure : P-9676-N
191 Anal Procedure : EAL-fis-2346n
192
193 Sample # : 880216-304
194 Operator badge # : 13164
195 Analysis name : N

196 Limits exceeded :
197 Results : 0.305
198 Error :
199 Units : UG/ML
200 Prep Procedure : P-9676-N
201 Anal Procedure : EAL-fis-2346n
202
203 Sample # : 880216-305
204 Operator badge #: 13164
205 Analysis name : N
206 Limits exceeded :
207 Results : 0.191
208 Error :
209 Units : UG/ML
210 Prep Procedure : P-9676-N
211 Anal Procedure : EAL-fis-2346n
212
213 Sample # : 880216-307
214 Operator badge #: 13164
215 Analysis name : N
216 Limits exceeded :
217 Results : 0.227
218 Error :
219 Units : UG/ML
220 Prep Procedure : P-9676-N
221 Anal Procedure : EAL-fis-2346n
222
223 Sample # : 880216-308
224 Operator badge #: 13164
225 Analysis name : N
226 Limits exceeded :
227 Results : 0.190
228 Error :
229 Units : UG/ML
230 Prep Procedure : P-9676-N
231 Anal Procedure : EAL-fis-2346n
232
233 Sample # : 880216-309
234 Operator badge #: 13164
235 Analysis name : N
236 Limits exceeded :
237 Results : 0.116
238 Error :
239 Units : UG/ML
240 Prep Procedure : P-9676-N
241 Anal Procedure : EAL-fis-2346n
242
243 Sample # : 880310-023
244 Operator badge #: 13164
245 Analysis name : N
246 Limits exceeded :

247 Results : 0.114
248 Error :
249 Units : UG/ML
250 Prep Procedure : P-9676-N
251 Anal Procedure : EAL-fis-2346n
252
253 Sample # : 880310-024
254 Operator badge #: 13164
255 Analysis name : N
256 Limits exceeded :
257 Results : 0.374
258 Error :
259 Units : UG/ML
260 Prep Procedure : P-9676-N
261 Anal Procedure : EAL-fis-2346n
262
263 Sample # : 880310-025
264 Operator badge #: 13164
265 Analysis name : N
266 Limits exceeded :
267 Results : 0.272
268 Error :
269 Units : UG/ML
270 Prep Procedure : P-9676-N
271 Anal Procedure : EAL-fis-2346n
272
273 Sample # : 880310-025
274 Operator badge #: 13164
275 Analysis name : N
276 Limits exceeded :
277 Results : 0.279
278 Error :
279 Units : UG/ML
280 Prep Procedure : P-9676-N
281 Anal Procedure : EAL-fis-2346n
282
283 Sample # : 880420-056
284 Operator badge #: 13164
285 Analysis name : N
286 Limits exceeded : <
287 Results : 0.020
288 Error :
289 Units : UG/ML
290 Prep Procedure : N-123
291 Anal Procedure : EAL-fis-9763
292
293 Sample # : 880420-057
294 Operator badge #: 13164
295 Analysis name : N
296 Limits exceeded : <
297 Results : 0.020

298 Error :
299 Units : UG/ML
300 Prep Procedure : N-123
301 Anal Procedure : EAL-fis-9763
302
303 Sample # : 880411-051
304 Operator badge #: 13164
305 Analysis name : N
306 Limits exceeded :
307 Results : 0.540
308 Error :
309 Units : UG/ML
310 Prep Procedure : N-123
311 Anal Procedure : EAL-fis-9763
312
313 Sample # : 880310-026
314 Operator badge #: 13164
315 Analysis name : P
316 Limits exceeded :
317 Results : 0.118
318 Error :
319 Units : UG/ML
320 Prep Procedure :
321 Anal Procedure :
322
323 Sample # : 880310-026
324 Operator badge #: 13164
325 Analysis name : P
326 Limits exceeded :
327 Results : 0.067
328 Error :
329 Units : UG/ML
330 Prep Procedure :
331 Anal Procedure :
332
333 Sample # : 880310-027
334 Operator badge #: 13164
335 Analysis name : P
336 Limits exceeded :
337 Results : 0.075
338 Error :
339 Units : UG/ML
340 Prep Procedure :
341 Anal Procedure :
342
343 Sample # : 880310-028
344 Operator badge #: 13164
345 Analysis name : P
346 Limits exceeded :
347 Results : 0.101
348 Error :

349 Units : UG/ML
350 Prep Procedure :
351 Anal Procedure :
352
353 Sample # : 880310-029
354 Operator badge #: 13164
355 Analysis name : P
356 Limits exceeded :
357 Results : 0.077
358 Error :
359 Units : UG/ML
360 Prep Procedure :
361 Anal Procedure :
362
363 Sample # : 880310-040
364 Operator badge #: 13164
365 Analysis name : P
366 Limits exceeded :
367 Results : 0.122
368 Error :
369 Units : UG/ML
370 Prep Procedure :
371 Anal Procedure :
372
373 Sample # : 880310-041
374 Operator badge #: 13164
375 Analysis name : P
376 Limits exceeded :
377 Results : 0.043
378 Error :
379 Units : UG/ML
380 Prep Procedure :
381 Anal Procedure :
382
383 Sample # : 880310-043
384 Operator badge #: 13164
385 Analysis name : P
386 Limits exceeded :
387 Results : 0.117
388 Error :
389 Units : UG/ML
390 Prep Procedure :
391 Anal Procedure :
392
393 Sample # : 880310-047
394 Operator badge #: 13164
395 Analysis name : P
396 Limits exceeded :
397 Results : 0.103
398 Error :
399 Units : UG/ML

400 Prep Procedure :
401 Anal Procedure :
402
403 Sample # : 880420-037
404 Operator badge #: 13164
405 Analysis name : ammonia as ion
406 Limits exceeded : <
407 Results : 0.064
408 Error :
409 Units : UG/ML
410 Prep Procedure :
411 Anal Procedure :
412
413 Sample # : 880420-038
414 Operator badge #: 13164
415 Analysis name : ammonia as ion
416 Limits exceeded : <
417 Results : 0.064
418 Error :
419 Units : UG/ML
420 Prep Procedure :
421 Anal Procedure :
422
423 Sample # : 880420-039
424 Operator badge #: 13164
425 Analysis name : ammonia as ion
426 Limits exceeded : <
427 Results : 0.064
428 Error :
429 Units : UG/ML
430 Prep Procedure :
431 Anal Procedure :
432
433 Sample # : 880420-040
434 Operator badge #: 13164
435 Analysis name : ammonia as ion
436 Limits exceeded :
437 Results : 0.076
438 Error :
439 Units : UG/ML
440 Prep Procedure :
441 Anal Procedure :
442
443 Sample # : 880420-041
444 Operator badge #: 13164
445 Analysis name : ammonia as ion
446 Limits exceeded :
447 Results : 0.100
448 Error :
449 Units : UG/ML
450 Prep Procedure :

451 Anal Procedure :
452
453 Sample # : 880420-042
454 Operator badge #: 13164
455 Analysis name : ammonia as ion
456 Limits exceeded : <
457 Results : 0.064
458 Error :
459 Units : UG/ML
460 Prep Procedure :
461 Anal Procedure :
462
463 Sample # : 880420-055
464 Operator badge #: 13164
465 Analysis name : ammonia as ion
466 Limits exceeded : <
467 Results : 0.064
468 Error :
469 Units : UG/ML
470 Prep Procedure :
471 Anal Procedure :
472
473 Sample # : 880419-055
474 Operator badge #: 13164
475 Analysis name : N
476 Limits exceeded :
477 Results : 0.083
478 Error :
479 Units : UG/ML
480 Prep Procedure : N-123
481 Anal Procedure : EAL-fis-6663
482
483 Sample # : 880419-056
484 Operator badge #: 13164
485 Analysis name : N
486 Limits exceeded :
487 Results : 0.087
488 Error :
489 Units : UG/ML
490 Prep Procedure : N-123
491 Anal Procedure : EAL-fis-6663
492
493 Sample # : 880419-073
494 Operator badge #: 13164
495 Analysis name : N
496 Limits exceeded :
497 Results : 0.368
498 Error :
499 Units : UG/ML
500 Prep Procedure : N-123
501 Anal Procedure : EAL-fis-6663

502
503 Sample # : 880419-076
504 Operator badge #: 13164
505 Analysis name : N
506 Limits exceeded :
507 Results : 0.012
508 Error :
509 Units : UG/ML
510 Prep Procedure : N-123
511 Anal Procedure : EAL-fis-6663
512
513 Sample # : 880419-077
514 Operator badge #: 13164
515 Analysis name : N
516 Limits exceeded :
517 Results : 0.013
518 Error :
519 Units : UG/ML
520 Prep Procedure : N-123
521 Anal Procedure : EAL-fis-6663
522
523 Sample # : 880419-078
524 Operator badge #: 13164
525 Analysis name : N
526 Limits exceeded :
527 Results : 0.012
528 Error :
529 Units : UG/ML
530 Prep Procedure : N-123
531 Anal Procedure : EAL-fis-6663
532
533 Sample # : 880419-079
534 Operator badge #: 13164
535 Analysis name : N
536 Limits exceeded :
537 Results : 0.015
538 Error :
539 Units : UG/ML
540 Prep Procedure : N-123
541 Anal Procedure : EAL-fis-6663
542
543 Sample # : 880419-084
544 Operator badge #: 13164
545 Analysis name : N
546 Limits exceeded :
547 Results : 0.092
548 Error :
549 Units : UG/ML
550 Prep Procedure : N-123
551 Anal Procedure : EAL-fis-6663
552

553 Sample # : 880419-085
554 Operator badge #: 13164
555 Analysis name : N
556 Limits exceeded :
557 Results : 0.075
558 Error :
559 Units : UG/ML
560 Prep Procedure : N-123
561 Anal Procedure : EAL-fis-6663
562
563 Last Data : \$\$\$
564 Entries : 139
565 \$

Internal Distribution

1. B. R. Appleton
2. P. L. Howell
3. W. R. Laing
4. S. A. MacIntyre
5. H. S. McKown
- 6-10. T. R. Mueller
11. T. B. Shope
12. J. H. Stewart, Jr.
13. N. A. Teasley
14. Central Research Library
15. Document Reference Section
- 16-18. Laboratory Records
19. Laboratory Records - RC
20. Patent Office

External Distribution

- 21-30. Office of Scientific and Technical Information, U. S. Department of Energy, Oak Ridge, TN 37831
31. Office of Assistant Manager for Energy Research and Development, DOE-ORO, Oak Ridge, Tn. 37831