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AFS DETECTION LIMITS

Listing and explanation of a computer program for the Baird Plasma/AFS and Apple II computer to determine detection limits

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Abstract

AFS DETECTION LIMITS is a computer program written specifically for an Apple II PLUS computer with 48K of memory, one disk drive, and an Epson MX-80 printer. The computer is connected to a PLASMA/AFS Atomic Fluorescence Spectrometer manufactured by Baird Corporation. The program is menu driven and prompts the operator for all input. The program collects raw signal data from the PLASMA/AFS and then calculates, displays and prints the mean, standard deviation, and relative standard deviation of the signal data, and detection limit for each element determined in a standard solution. These statistics and detection limits are used to check instrument performance and to set up the operating conditions of the instrument. A data collection routine is also provided in the AFS DETECTION LIMITS program to collect and print data from the menu modes of the PLASMA/AFS instrument.

Introduction

The Atomic Fluorescence Spectrometer (PLASMA/AFS) manufactured by Baird Corporation is capable of determining from 1 to 12 elements simultaneously. The instrument has two modes of operation: (1) the menu mode allows for the calibration of each of the twelve channels of the instrument and the printout of results on an internal printer; and (2) the command mode provides raw signal data but has no provision for printing this raw data. The raw signal data are used to set up the instrument and calculate detection limits of elements in standard solutions. Detection limits are used to check for proper instrument performance and to determine the best instrumental parameters and plasma conditions to use. The detection limit is defined, in this report, as the concentration of an element that will produce a signal that is twice the standard deviation of ten repetitions of the signal produced by a blank.

The Baird PLASMA/AFS generates data rapidly but has no provision for printing raw data or calculating detection limits using the internal computer of the instrument. Because the raw signal data and detection limit information are used to set up the instrument, an external computer is useful, if not essential, for these data collections and calculations. By connecting an Apple II PLUS Computer to the external printer interface of the Baird PLASMA/AFS and using the program described in this report, detection limits and raw instrumental data can be collected and printed.

AFS DETECTION LIMITS is a computer program written specifically for an Apple II PLUS Computer with 48K of memory, one disk drive, and an Epson MX-80 printer. It is to be used to collect instrumental data from a Baird PLASMA/AFS and calculate detection limits of elements in standard solutions and has no other intended purpose. The program is menu driven and prompts the operator for all input. The program collects raw signal data from the Baird PLASMA/AFS, and then calculates, displays and prints the mean, standard deviation, relative standard deviation, and detection limit for each element in a standard solution. A data collection routine is also provided in the AFS DETECTION LIMITS program to collect and print data from the menu modes of the Baird PLASMA/AFS instrument. The user of this program must have a knowledge of the Baird PLASMA/AFS and its operation, however, little computer experience is necessary to use the program.

Program description

This program is written in Applesoft Basic Language for an Apple II PLUS computer system with 48K memory and one disk drive and an Epson MX-80 printer. The program is menu driven and prompts the operator for all input. All inputs use "Y" for yes, "N" for no, and "Return" for a default or no change. Other inputs are entered by pressing a numbered key, or if operator

input information is requested, by typing numbers or words followed by the "Return" key.

The program consists of three sections: input; data collection and reduction; and output.

The input section requires that the operator enter information in response to prompting menus, as they appear on the screen. The information entered is used in the data collection and reduction and output sections for labeling and heading information and for selecting data for manipulation using output routines provided. These "Header" conditions are stored on disk and are retrieved by the program; therefore, only minor changes are usually required in subsequent runs.

The data collection and reduction section of the program passes control of the computer to the Baird PLASMA/AFS instrument for data input. Data, for one to 12 elements, are transmitted from the test exerciser mode of the Baird PLASMA/AFS instrument to the Apple II computer. A maximum of 10 repetitions may be made on a maximum of 10 runs of a standard solution. Between data collection repetitions provision is made for the operator to abort the data collection and to reject data before they are used in the calculations performed by the program. The mean, standard deviation, relative standard deviation, and detection limit are calculated for each element in each standard solution run. The detection limit is calculated using the mean and standard deviation of the last blank run and the standards run by the formula:

$$D = \frac{2VC}{S-B}$$

Where, D is the detection limit, V is the standard deviation of the blank signal, C is the concentration of the standard, S is the mean standard signal, and B in the mean blank signal. The blank values used in the calculations are always the last ones run. The data collection routine displays or prints data from the menu modes of the PLASMA/AFS instrument.

The output section provides for display and/or printout of the data collected and calculated. Printer commands for the Epson MX-80 printer are embedded in the program to provide a readable and useful printout. Options are provided to allow the operator to print as much or as little of the header information as is needed to indicate the conditions under which the data were collected.

Program execution

The following are the prompts that appear on the computer screen, shown as underlined characters. A brief description of each prompt is given with the possible responses. The numbers in parentheses are the program line numbers at which these prompts occur.

HOW MANY ELEMENTS ARE YOU RUNNING? (210)

A number from 0 to 12 is entered and the return key pressed. If 0 is entered, the program goes directly to the ending routine. If a number greater than 12 is entered, the prompt will return.

SELECT PRINTER OPTION (240)
0= NOTHING
1= EVERYTHING

ENTER OPTION NUMBER

Only 0 or 1 will be accepted. If 0 is entered, nothing is printed. If 1 is entered, all data requested in the next menu are printed. The next menu appears as soon as a 0 or 1 is entered.

SELECT DATA OPTION (320)
0= ALL DATA FULL HEADER
1= ALL DATA ELEMENT INFO.
2= ALL DATA NO HEADER
3= DETECTION LIMITS FULL HEADER
4= DETECTION LIMITS ELEMENT INFO.
5= DETECTION LIMITS NO HEADER
6= DATA FROM KEYBOARD FULL HEADER
7= DATA FROM KEYBOARD ELEMENT INFO.
8= DATA FROM KEYBOARD NO HEADER
9= PRINT FROM MENU MODE

ENTER OPTION NUMBER (440)

When 0, 3, or 6 (full header) is selected, all information contained in the header file will be displayed or printed next to the titles shown in the next menu (title, operator, day, month, year, time, power, carrier flow, coolant flow, pump speed, remarks, remarks, remarks, and remarks). Likewise, if 1, 4, or 7 (element information) is chosen, that is all that will be displayed or printed under the titles of Position, Element, Current, and PMT. Entry of 6, 7, or 8 allows the operator to input data manually. Selection 9 provides the use of the computer and printer as an external printer from the menu modes of the instrument.

TITLE
OPERATOR
DAY
MONTH
YEAR
TIME
POWER
CARRIER FLOW
COOLANT FLOW
PUMP SPEED
REMARKS
REMARKS
REMARKS
REMARKS

DO YOU WANT TO CHANGE ANYTHING? (1700)

If a header was selected in the previous menu, any information contained in the header disk file will be displayed on the screen with each of the above titles (title, operator, day, month, year, time, power, carrier flow, coolant flow, pump speed, remarks, remarks, remarks, and remarks). If any key except "Y" is pressed, all of the information is retained and used in subsequent printouts. If "Y" is pressed, the following prompt is displayed on the screen, and each of the above titles (title, operator, day, month, year, time, power, carrier flow, coolant flow, pump speed, remarks, remarks, remarks, and remarks) is displayed one at a time with its current contents in inverse video.

RETURN FOR NO CHANGE < / > TO DELETE (1860)

As the prompt indicates, pressing the return key retains the contents of that section of the header as displayed in inverse video. If a "/" key is entered, that section is deleted and nothing will be displayed or printed in that position of the header. Anything typed into the keyboard and followed by the return key replaces the contents of that section. After a response is made to the last remark, the header, with changes, is once again displayed and can be accepted or further changed.

POSITION ELEMENT CURRENT PMT

DO YOU WANT TO CHANGE ANYTHING? (1860)

The contents of the element information file will be displayed under each of the headings (position, element, current, pmt) for the number of elements being run. If any key except "Y" is pressed, all of the above information is retained and used in subsequent printouts.

If "Y" is entered, the following message is displayed, and each of the above titles (position, element, current, pmt) is displayed, one at a time, with its contents in inverse video.

RETURN FOR NO CHANGE < / > TO DELETE (1860)

As the prompt indicates, pressing the return key retains the contents of that section of the header as displayed in inverse video. If a "/" key is entered, that section is deleted and nothing will be displayed or printed in that position of the header. Anything typed into the keyboard and followed by the return key replaces the contents of that section. After responding to the last PMT (photomultiplier tube voltage), the header, as changed, is once again displayed and can be accepted or altered. The positions of the elements can be entered in any order but they must be in the range of 1 to 12 and be the module positions in use by the AFS instrument. The program will not accept two positions with the same number or two elements with the same symbol.

HOW MANY REPETITIONS DO YOU WANT? (2130)

The number of repeats desired is entered. The range must be from 0 to 10 or an error message will be displayed and the question will be asked again. If 0 is entered, the program will go to the end of data input section and ask if more standards are to be run. If a number between 1 and 10 is entered, the program continues.

ENTER REMARK FOR THIS RUN (2160)

A remark of up to 255 characters can be entered for the run. The return key is pressed, if no remark is desired.

FOR RUN " "

IS CONCENTRATION = FOR ALL ELEMENTS (2160)

The return key or "Y" is pressed if the standard to be run contains all of the elements at the same concentration. The prompt below (WHAT IS THE

CONCENTRATION IN G/ML?) appears. If the standard to be run contains the elements at different concentrations, then "N" is entered and the second prompt (ENTER CONCENTRATION IN G/ML FOR ELEMENT " ") appears.

WHAT IS THE CONCENTRATION IN G/ML: (2170)

A concentration value that equals the standard is entered. If the solution is a blank, then 0 is entered.

ENTER CONCENTRATION IN G/ML FOR ELEMENT " " (2190)

This prompt will appear for each element being run and requires that a concentration be entered for each.

DO YOU HAVE ANY CHANGES? (2220)

If "Y" is entered, the program returns to the prompt, "HOW MANY REPETITIONS DO YOU WANT?", and all entries must be re-entered. If the return key is pressed, all entries are accepted and the program continues by going directly to accepting data from the instrument or keyboard. The instrument must be in the test exerciser mode with the external print command given. Control of the computer is taken away from the operator until data are transferred from the instrument to the computer. At that time the following message appears and "*" are slowly printed across the screen.

HIT CTRL C TO ABORT: RUN " " OF " " (2310)

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****

The run and the data taken in the run can be canceled by pressing the CTRL and C keys simultaneously, while the "*" are being printed across the screen. The program then returns to the prompt, "HOW MANY REPETITIONS DO YOU WANT?", and the run can be restarted. If the data collection is not aborted, the data are collected for the number of repeats selected. The computer will beep and the following prompt will appear.

RUN " " OF " " DONE CHANGE STANDARDS! (2300)

The computer will take some time making calculations before printing the newly calculated data on the screen. Then the following prompt will be displayed.

DO YOU HAVE MORE STANDARDS TO RUN? (2640)

If the return key is pressed, the program will ask for the number of repetitions for the next run and go through the same data collection routine. If "N" is entered, the data selected will be printed on the printer. If no printout was selected, the data will be printed on the screen. The following prompt will be displayed after the print.

DO YOU WANT TO CONTINUE USING THE SAME ELEMENTS AND SAME DATA? (3130)

If "Y" is entered, then the next prompt appears. If the return key is pressed, the second prompt appears.

DO YOU WANT TO CHANGE PRINT INSTRUCTIONS? (3140)

If "Y" is entered, then the program returns to the beginning, prompts for changes, except the number of elements which cannot be changed. If any other key is entered, the program returns to the prompt, "DO YOU HAVE MORE STANDARDS TO RUN?".

DO YOU WANT TO RUN NEW DATA? (3160)

If "Y" is entered, the program starts from the beginning. If any other key is entered, the next prompt appears.

DO YOU WANT TO QUIT? (3190)

If any key other than "Y" is pressed, the program returns to the ending prompts starting at "DO YOU WANT TO CONTINUE USING THE SAME ELEMENTS AND SAME DATA?". If "Y" is entered, the following prompt appears.

ATOMIC FLUORESCENCE PROGRAM ENDED! ENTER RUN TO BEGIN AGAIN (3200)

A Computer listing of the AFS DETECTION LIMITS program

```
100  REM  THIS  PROGRAM  COLLECTS  DATA  FROM  THE  BAIRD  ATOMIC
FLUORESCENCE ICP CALCULATES STATISTICS, AND DETECTION LIMITS.
110  REM   PROVISION IS MADE TO USE THE COMPUTER AND PRINTER AS AN
EXTERNAL PRINTER
120  REM    LAST UPDATED ON 11 JANUARY 1984
130  REM  WRITTEN BY ALLEN MEIER AFTER A PROGRAM OF ROBERT BIGELOW
OF USGS DENVER, CO
140  REM  ************************
150  REM **PRINTER MX-80 EPSON**
160  REM   ************************
170      DIM      Z$(12),   B$(12),  C$(12),  D$(12,10),  A$(100),
EL(12,10,10), RS(12,10), SQ(12,10), ST(12,10), SU(12,10), EL$(12),
LC$(12),  PM$(12),   MP$(12),   D(12,10),   ME(12,10),   C(12,10),
RS$(12,10), ST%(12,10), ME%(12,10), E$(12)
180 D$ =  CHR$ (4)
190  HOME
200  RESTORE
210  INPUT "HOW MANY ELEMENTS ARE YOU  RUNNING?";  NE:  IF  NE = 0
GOTO 3190
220  DATA    "A","B","C","D","E","F","G","H","I","J","K","L"
230  FOR N = 1 TO NE: READ NE$: NEXT
240    HOME  :  INVERSE  : PRINT "SELECT PRINTER OPTION": NORMAL :
PRINT
250  ONERR  GOTO 240
260  PRINT : PRINT "0=  NOTHING "
270  PRINT : PRINT "1=  EVERYTHING "
280  PRINT : PRINT : INVERSE : PRINT "ENTER OPTION NUMBER": NORMAL
290  GET A: POKE 216,0
300  A = A + 1
310  IF A > 3 GOTO 240
320  HOME : INVERSE : PRINT "SELECT DATA OPTION": NORMAL : PRINT
330  ONERR  GOTO 320
340  PRINT : PRINT "0=  ALL DATA  FULL HEADER"
350  PRINT : PRINT "1=  ALL DATA  ELEMENT INFO."
360  PRINT : PRINT "2=  ALL DATA  NO HEADER"
370  PRINT : PRINT "3=  DETECTION LIMITS  FULL HEADER"
380  PRINT : PRINT "4=  DETECTION LIMITS  ELEMENT INFO."
390  PRINT : PRINT "5=  DETECTION LIMITS NO HEADER"
400  PRINT : PRINT "6=  DATA FROM KEYBOARD  FULL HEADER"
410  PRINT : PRINT "7=  DATA FROM KEYBOARD  ELEMENT INFO."
420  PRINT : PRINT "8=  DATA FROM KEYBOARD NO HEADER"
430  PRINT : PRINT "9=  PRINT FROM MENU MODE"
440  PRINT : PRINT : INVERSE : PRINT "ENTER OPTION NUMBER": NORMAL
450  GET H: POKE 216,0
460  H = H + 1
470  IF H > 10 GOTO 240
480  ON H GOTO 490,550,550,490,550,550,490,550,550,3710
490  ONERR  GOTO 530
500  PRINT D$: PRINT D$;"OPEN HEADFILE"
510  PRINT D$;"READ HEADFILE"
```

```
520  INPUT TI$, OP$, DA$,  MO$,  YR$, T$, PO$, CA$, CO$, RE$, OX$,
PU$, R1$, R2$, R3$, R4$
530  PRINT D$;"CLOSE HEADFILE"
540  POKE 216,0
550  ONERR  GOTO 610
560  PRINT D$: PRINT D$;"OPEN";NE$
570  PRINT D$;"READ";NE$
580  INPUT NE
590  FOR I = 1 TO NE: INPUT EL$(I),MP$(I),LC$(I),PM$(I)
600  NEXT  O  PRINT D$;"CLOSE";NE$
620  POKE 216,0
630  GOTO 1490
640  HOME : ON H GOTO 680, 1070, 1070, 680, 1070, 1070, 680, 1070,
1070, 3710
650  REM ********************
660  REM *HEADER INPUT*
670  REM ********************
680  PRINT "TITLE  ";
690   INVERSE  :  PRINT TI$: NORMAL : INPUT X$: IF X$ <  > "" THEN
TI$ = X$: IF X$ = "/" THEN TI$ = ""
700  PRINT "OPERATOR  ";
710  INVERSE : PRINT  OP$:  NORMAL  : INPUT X$: IF X$ <  > "" THEN
OP$ = X$: IF X$ = "/" THEN OP$ = ""
720  PRINT "DAY  ";
730  INVERSE : PRINT DA$: NORMAL : INPUT X$:  IF  X$  <  > "" THEN
DA$ = X$: IF X$ = "/" THEN DA$ = ""
740  PRINT "MONTH  ";
750   INVERSE  :  PRINT MO$: NORMAL : INPUT X$: IF X$ <  > "" THEN
MO$ = X$: IF X$ = "/" THEN MO$ = ""
760  PRINT "YEAR  ";
770  INVERSE : PRINT YR$: NORMAL :  INPUT  X$:  IF X$ <  > "" THEN
YR$ = X$: IF X$ = "/" THEN YR$ = ""
780  PRINT "TIME  ";
790  INVERSE : PRINT T$: NORMAL : INPUT X$: IF X$  <  > "" THEN T$
= X$: IF X$ = "/" THEN T$ = ""
800  PRINT "POWER  ";
810  INVERSE : PRINT PO$:  NORMAL  :  INPUT X$: IF X$ <  > "" THEN
PO$ = X$: IF X$ = "/" THEN PO$ = ""
820  PRINT "CARRIER FLOW  ";
830   INVERSE  :  PRINT CA$: NORMAL : INPUT X$: IF X$ <  > "" THEN
CA$ = X$: IF X$ = "/" THEN CA$ = ""
O  PRINT "COOLANT FLOW  ";
850  INVERSE : PRINT  CO$:  NORMAL  : INPUT X$: IF X$ <  > "" THEN
CO$ = X$: IF X$ = "/" THEN CO$ = ""
860  PRINT "REDUCTANT FLOW  ";
870  INVERSE : PRINT RE$: NORMAL : INPUT X$:  IF  X$  <  > "" THEN
RE$ = X$: IF X$ = "/" THEN RE$ = ""
880  PRINT "OXIDANT FLOW  ";
890   INVERSE  :  PRINT OX$: NORMAL : INPUT X$: IF X$ <  > "" THEN
OX$ = X$: IF X$ = "/" THEN OX$ = ""
900  PRINT "PUMP SPEED  ";
910  INVERSE : PRINT PU$: NORMAL :  INPUT  X$:  IF X$ <  > "" THEN
PU$ = X$: IF X$ = "/" THEN PU$ = ""
920  PRINT "REMARKS  ";
```

```
930  INVERSE : PRINT R1$: NORMAL : INPUT X$: IF X$  <    > "" THEN
R1$ = X$: IF X$ = "/" THEN R1$ = ""
940  PRINT "REMARKS  ";
950  INVERSE : PRINT R2$:  NORMAL  :  INPUT X$: IF X$ <  > "" THEN
R2$ = X$: IF X$ = "/" THEN R2$ = ""
960  PRINT "REMARKS  ";
970   INVERSE  :  PRINT R3$: NORMAL : INPUT X$: IF X$ <  > "" THEN
R3$ = X$: IF X$ = "/" THEN R3$ = ""
980  PRINT "REMARKS  ";
990  INVERSE : PRINT  R4$:  NORMAL  : INPUT X$: IF X$ <  > "" THEN
R4$ = X$: IF X$ = "/" THEN R4$ = ""
1000  REM ********************
1010  REM *END HEADER INPUT*
1020  REM ************************
1030  POKE 34,0: HOME : GOTO 1550
1040  REM ********************
1050  REM *ELEMENT INFOR INPUT*
1060  REM ************************
1070  IF NE = 0 THEN  GOTO 1200
1080  FOR I = 1 TO NE
1090  PRINT "MODULE POSITION  ";
1100  INVERSE : PRINT MP$(I): NORMAL : INPUT X$:  IF  X$  <   > ""
THEN MP$(I) = X$: IF X$ = "/" THEN MP$(I) = ""
1110  IF  VAL (MP$(I)) > 12 THEN  FLASH : GOTO 1090
1120  IF  VAL (MP$(I)) <  = 0 THEN  FLASH : GOTO 1090
1130  PRINT "ELEMENT ";
1140   INVERSE  :  PRINT  EL$(I): NORMAL : INPUT X$: IF X$ <  > ""
THEN EL$(I) = X$: IF X$ = "/" THEN EL$(I) = ""
1150  PRINT "LAMP CURRENT  ";
1160  INVERSE : PRINT LC$(I): NORMAL :  INPUT  X$:  IF  X$ <  > ""
THEN LC$(I) = X$: IF X$ = "/" THEN LC$(I) = ""
1170  PRINT "PHOTOMULTIPLIER SETTING  ";
1180  INVERSE : PRINT PM$(I): NORMAL : INPUT X$: IF X$  <    >  ""
THEN PM$(I) = X$: IF X$ = "/" THEN PM$(I) = ""
1190  NEXT
1200  HOME
1210  FOR I = 1 TO NE
1220  FOR X = 1 TO NE
1230  IF I = X THEN  GOTO 1260
1240  IF MP$(I) = MP$(X)  THEN   POKE 34,0: HOME : FLASH : PRINT "
MODULE POSITION ";MP$(I);" USED TWICE!": NORMAL : GOTO 1750
1250   IF  EL$(I) = EL$(X) THEN  POKE 34,0: HOME : FLASH : PRINT "
ELEMENT ";EL$(I);" USED TWICE!": NORMAL : GOTO 1750
1260  NEXT
1270  NEXT
1280  FOR I = 1 TO 12
1290  Z =  VAL (MP$(I))
1300  Z$(Z) = MP$(I)
1310  B$(Z) = EL$(I)
1320  C$(Z) = LC$(I)
1330  E$(Z) = PM$(I)
1340  NEXT
1350  X = 1
1360  FOR I = 1 TO 12
1370  IF Z$(I) = "" THEN  GOTO 1440
```

```
1380  MP$(X) = Z$(I)
1390  EL$(X) = B$(I)
1400  LC$(X) = C$(I)
1410  PM$(X) = E$(I)
1420  X = X + 1
1430  Z$(I) = ""
1440  NEXT
1450  POKE 34,0: HOME
1460  REM ********************
1470  REM END ELEMENT INFO INPUT*
1480  REM ***********************
1490  HOME : ON  H GOSUB 1550, 1750, 1750, 1550, 1750, 1750, 1550,
1750, 1750, 3710
1500  IF BB <  > 1 GOTO 2120
1510  GOTO 1910
1520  REM ***********************
1530  REM *HEADER OUTPUT*
1540  REM ********************
1550  IF TI$ <  > "" THEN  PRINT "TITLE  ";TI$
1560  IF OP$ <  > "" THEN  PRINT "OPERATOR  ";OP$
1570  IF (DA$ <  > "") AND (MO$  <    > "") AND (YR$ <  > "") THEN
PRINT "DATE  ";DA$;" ";MO$;" ";YR$;
1580  IF T$ <  > "" THEN  PRINT "     TIME  ";T$
1590  IF T$ = "" THEN  PRINT
1600  IF PO$ <  > "" THEN  PRINT "POWER  ";PO$
1610  IF CA$ <  > "" THEN  PRINT "CARRIER FLOW  ";CA$
1620  IF CO$ <  > "" THEN  PRINT "COOLANT FLOW  ";CO$
1630  IF RE$ <  > "" THEN  PRINT "REDUCTANT FLOW  ";RE$
1640  IF OX$ <  > "" THEN  PRINT "OXIDANT FLOW  ";OX$
1650  IF PU$ <  > "" THEN  PRINT "PUMP SPEED  ";PU$
1660  IF R1$ <  > "" THEN  PRINT "REMARKS  ";R1$
1670  IF R2$ <  > "" THEN  PRINT "REMARKS  ";R2$
1680  IF R3$ <  > "" THEN  PRINT "REMARKS  ";R3$
1690  IF R4$ <  > "" THEN  PRINT "REMARKS  ";R4$
1700  INPUT "DO YOU WANT TO CHANGE ANYTHING?";B$: IF B$ = "Y" THEN
BB =  1:  INVERSE  : PRINT "RETURN FOR NO CHANGE < / > TO DELETE":
NORMAL : PRINT : POKE 34, PEEK (37): GOTO 640
1710  REM ********************
1720  REM *HEADER OUT END*
1730  REM ********************
1740  POKE 34,0: HOME
1750  PRINT "POSITION  ELEMENT  CURRENT  PMT"
1760  REM ********************
1770  REM **ELEMENT OUT**
1780  REM ********************
1790  FOR I = 1 TO NE
1800  HTAB 4: PRINT MP$(I);
1810  HTAB 13: PRINT EL$(I);
1820  HTAB 22: PRINT LC$(I);
1830  HTAB 30: PRINT PM$(I)
1840  NEXT
1850  P =  FRE (0)
1860  INPUT "DO YOU WANT TO CHANGE ANYTHING?";B$: IF B$ = "Y" THEN
BB = 1: INVERSE : PRINT "RETURN FOR  NO  CHANGE  < / > TO DELETE":
NORMAL : PRINT : POKE 34, PEEK (37): GOTO 1070
```

```
1870  RETURN
1880  REM ********************
1890  REM  **DISK HEADER FILES**
1900  REM ********************
1910  ON H GOTO 1920,1980,1980,1920,1980,1980,1920,1980,1980,3710
1920  PRINT D$;"OPEN HEADFILE"
1930  PRINT D$;"DELETE HEADFILE"
1940  PRINT D$;"OPEN HEADFILE"
1950  PRINT D$;"WRITE HEADFILE"
1960  PRINT TI$: PRINT OP$: PRINT DA$: PRINT MO$: PRINT YR$: PRINT
T$:  PRINT  PO$: PRINT CA$: PRINT CO$: PRINT RE$: PRINT OX$: PRINT
PU$: PRINT R1$: PRINT R2$: PRINT R3$: PRINT R4$
1970  PRINT D$;"CLOSE HEADFILE"
1980  IF BB <  > 1 GOTO 2120
1990  PRINT D$;"OPEN";NE$
2000  PRINT D$;"DELETE";NE$
2010  PRINT D$;"OPEN";NE$
2020  PRINT D$;"WRITE";NE$
2030  PRINT NE
2040  FOR I = 1  TO  NE: PRINT EL$(I): PRINT MP$(I): PRINT LC$(I):
PRINT PM$(I)
2050  NEXT
2060  PRINT D$;"CLOSE";NE$
2070  BB = 0
2080  REM ********************
2090  REM  **DISK HEADER END**
2100  REM **STAT. INITIALIZATION **
2110  REM **********************
2120  RN = RT + 1:RT = RT + 1
2130   SPEED=  255: PRINT : PRINT : INPUT "HOW MANY REPETITIONS DO
YOU WANT?  ";R(RN): IF  R(RN)  =  0  THEN RN = RT - 1:RT = RT - 1:
GOTO 2640
2140  IF R(RN) > 10 THEN  INVERSE :  PRINT "REPETITIONS MUST BE 10
OR LESS.": NORMAL : GOTO 2130
2150  PRINT : PRINT "ENTER REMARK FOR THIS RUN": INPUT R$(RN)
2160     PRINT   :  HTAB  14:  PRINT  "FOR  RUN  ";RN:  PRINT  "IS
CONCENTRATION = FOR ALL ELEMENTS?": GET B$
2170  PRINT : PRINT : PRINT :  IF B$ <  > "N" THEN  INPUT "WHAT IS
THE  CONCENTRATION  IN  UG/ML?";CC:  FOR I = 1 TO NE:C(I,RN) = CC:
NEXT : GOTO 2220
2180  FOR I = 1 TO NE
2190  PRINT : PRINT "ENTER  CONCENTRATION  IN  UG/ML  FOR  ELEMENT
";EL$(I);
2200  INPUT C(I,RN)
2210  NEXT
2220   PRINT  :  PRINT "DO YOU HAVE ANY CHANGES?": GET B$: IF B$ =
"Y" GOTO 2130
2230  ON H GOTO 2240,2240,2240,2240,2240,2240,3260,3260,3260,3710
2240  ONERR  GOTO 2130
2250  FOR I = 1 TO R(RN)
2260  REM ********************
2270  REM **INSTRUMENT INPUT**
2280  REM **********************
2290  PRINT D$: PRINT  D$;"IN#2": INPUT "";A$(I): PRINT D$;"IN#0":
IF A$(I) = "" THEN I = I - 1
```

```
2300   IF I = R(RN) THEN  PRINT   CHR$  (7),  CHR$  (7):  PRINT  :
INVERSE  :   PRINT   "RUN   ";I;"   OF  ";R(RN);"  DONE  ";"CHANGE
STANDARDS!": NORMAL : GOTO 2330
2310  PRINT "HIT CTRL C TO ABORT!  ";"RUN ";I;" OF ";R(RN)
2320  FOR Z = 0 TO 79: SPEED= 10: PRINT "*";: NEXT : SPEED= 255
2330  IF  LEN (A$(I)) < 10  *  NE  THEN  A$(I) = " " + A$(I): GOTO
2330
2340  FOR N = 1 TO NE
2341  L = ((N - 1) * 10) + 1
2343  FOR J = L TO L + 9
2344  IF ( MID$ (A$(I),J,1) = "-") THEN SIGN =  - 1
2350  NEXT
2360  REM  **********************
2370  REM  **STATISTICS CALCULATION**
2380  REM  **********************
2390  EL(N,RN,I) =  VAL ( MID$ (A$(I),L,10)) * SIGN
2400  SUM(N,RN) = SUM(N,RN) + EL(N,RN,I)
2401  SQ(N,RN) = SQ(N,RN) + EL(N,RN,I) ^ 2
2402  NEXT
2403  NEXT
2404  P =  FRE (0)
2405  POKE 216,0
2410  FOR N = 1 TO NE
2420  MEAN(N,RN) = SU(N,RN) / R(RN)
2430  IF R(RN) - 1 = 0 GOTO 2470
2440  IF ((SQ(N,RN) - ((SU(N,RN) ^ 2) / R(RN))) / (R(RN)  -  1)) <
= 0 GOTO 2470
2450  STDV(N,RN) =  SQR  ((SQ(N,RN)  - ((SU(N,RN) ^ 2) / R(RN))) /
(R(RN) - 1))
2460  RSD(N,RN) = ST(N,RN) * 100 / ME(N,RN)
2470   PRINT "ELEMENT ";EL$(N);"  RUN NUMBER= ";RN;"  REPETITIONS=
";R(RN);" CONC.= "C(N,RN);"  "R$(RN)
2475  ST%(N,RN) = ST(N,RN)
2476  RS$(N,RN) =  STR$ (RS(N,RN))
2480  IF ME(N,RN) >  32767  THEN   PRINT "MEAN= ";ME(N,RN);"  STD.
DEV.= ";ST%(N,RN);"  RSD%= "; LEFT$ (RS$(N,RN),4): GOTO 2510
2490  ME%(N,RN) = ME(N,RN)
2500  PRINT "MEAN=  ";ME%(N,RN);"  STD.DEV.= ";ST%(N,RN);"   RSD%=
"; LEFT$ (RS$(N,RN),4)
2510  NEXT
2520  IF RT < 2 THEN  INVERSE :  PRINT  "  NOT ENOUGH STANDARDS TO
RUN DETECTION LIMITS!": NORMAL : GOTO 2640
2530  FOR RN = 1 TO RT
2540  FOR I = 1 TO NE
2550  C = C + C(I,RN)
2551  NEXT  2552  IF C = 0 THEN B = RN
2560  C = 0
2570  NEXT
2580   IF  B  =  0 THEN  INVERSE : PRINT "NO BLANK HAS BEEN RUN!":
NORMAL : GOTO 2640
2590  FOR RN = 1 TO RT
2591  FOR N = 1 TO NE
2592  IF C(N,RN) = 0 GOTO 2630
2600  IF ME(N,RN) - ME(N,B) = 0 THEN D(N,RN) = 0: GOTO 2630
2610  D(N,RN) = (2000 * C(N,RN) * ST(N,B)) / (ME(N,RN) - ME(N,B))
```

```
2620  D$(N,RN) =  STR$ (D(N,RN))
2630  NEXT : NEXT
2640  PRINT  CHR$ (7): PRINT "DO YOU HAVE MORE STANDARDS TO RUN?":
GET B$: IF B$ <  > "N" GOTO 2120
2650  IF RT = 0 THEN  INVERSE  :  PRINT  "NO  STANDARDS HAVE BEEN
RUN!!": NORMAL : GOTO 3130
2660  IF A = 1 GOTO 3130
2670  IF A = 2 THEN  PRINT D$: PRINT D$;"PR#1"
2680  ON H GOSUB 3370,3370,2780,3370,3370,2900,3370,3370,2780,3710
2710  ON H GOSUB 2780,2780,2900,2900,2900,2900,2780,2780,2900,3710
2740  ON H GOTO 3090,3090,3090,2960,2960,2960,3090,3090,3090,3710
2750  REM   ***************
2760  REM   *DATA PRINT*
2770  REM   **********************
2780  FOR N = 1 TO NE
2790  FOR RN = 1 TO RT
2800    PRINT   CHR$ (18)"ELEMENT "; CHR$ (14);EL$(N); CHR$ (20);"
RUN=";RN;" REPS.=";R(RN);" CONC.=";C(N,RN);" UG/ML";
2810    IF  ME(N,RN)  > 32767  THEN    PRINT  "  MEAN=";ME(N,RN);"
STD.DEV.=";ST%(N,RN);" RSD%="; LEFT$ (RS$(N,RN),4): GOTO 2830
2820   PRINT  "  MEAN=";ME%(N,RN);" STD.DEV.=";ST%(N,RN);" RSD%=";
LEFT$ (RS$(N,RN),4)
2830  IF R$(RN) <  > "" THEN  PRINT R$(RN)
2840  IF C(N,RN) <  > 0 THEN  PRINT  CHR$ (14);"DET. LMT. "; LEFT$
(D$(N,RN),6);" UG/L "; CHR$ (20);
2850  PRINT  CHR$ (15);"RAW DATA ";
2860  FOR I = 1 TO R(RN): PRINT EL(N,RN,I);"  ";
2870  NEXT
2880  PRINT : NEXT : PRINT : NEXT
2890  PRINT  CHR$ (18)
2900  RETURN
2910  REM  ***************
2920  REM  *END OF DATA PRINT*
2930  REM  ***************
2940  REM  *DETECTION LIMIT PRINT*
2950  REM  ***************
2960  IF RT <  2  THEN   INVERSE : PRINT " NOT ENOUGH STANDARDS TO
RUN DETECTION LIMITS!": NORMAL : GOTO 3130
2970  FOR RN = 1 TO RT
2980  FOR I = 1 TO NE
2990  C = C + C(I,RN)
2991  NEXT
2992  IF C = 0 THEN B = RN
3000  C = 0
3010  NEXT
3020  IF B = 0 THEN  INVERSE :  PRINT  "NO  BLANK  HAS BEEN RUN!":
NORMAL : GOTO 3130
3030  FOR RN = 1 TO RT
3031  FOR N = 1 TO NE
3032  IF C(N,RN) = 0 GOTO 3080
3040  IF ME(N,RN) - ME(N,B) = 0 THEN D(N,RN) = 0: GOTO 3060
3050  D(N,RN) = (2000 * C(N,RN) * ST(N,B)) / (ME(N,RN) - ME(N,B))
3060  D$(N,RN) =  STR$ (D(N,RN))
```

```
3070  IF C(N,RN) < > 0 THEN PRINT CHR$ (18);"DET. LMT. AT
CONC.=";C(N,RN)" FOR "; CHR$ (14);EL$(N); CHR$ (20);" IS  "; LEFT$
(D$(N,RN),6);" UG/L ";R$(RN)
3080  NEXT : NEXT
3090  PRINT D$;"PR#0"
3100  REM  ********************
3110  REM  *END DETECTION LIMITS*
3120  REM  ********************
3130   PRINT  :  HTAB  8: PRINT "DO YOU WANT TO CONTINUE":  PRINT
"USING THE SAME ELEMENTS AND SAME DATA?": GET B$
3140  IF B$ = "Y"  THEN   PRINT  "DO  YOU  WANT  TO  CHANGE PRINT
INSTRUCTIONS? ": GET X$: IF X$ = "Y" THEN  GOTO 240
3150  IF B$ = "Y" GOTO 2640
3160   PRINT  :  PRINT : PRINT "DO YOU WANT TO RUN NEW DATA?": GET
B$: IF B$ < > "Y" GOTO 3190
3170  IF A < > 2 THEN  PRINT : CLEAR : GOTO 170
3180  IF B$ =  "Y"  THEN   PRINT D$: PRINT D$;"PR#1": PRINT  CHR$
(12): PRINT D$;"PR#0": CLEAR : GOTO 170
3190  PRINT : PRINT : PRINT "DO YOU WANT  TO QUIT?": GET B$: IF B$
< > "Y" THEN  GOTO 3220
3200   IF  A  <  > 2 THEN  PRINT : HOME : PRINT D$;"PR#0": PRINT
"ATOMIC FLUORESCENCE PROGRAM ENDED!": PRINT : PRINT " ENTER RUN TO
BEGIN AGAIN": END
3210  IF B$ = "Y" THEN  PRINT  D$:  PRINT  D$;"PR#1": PRINT  CHR$
(12):  HOME  : PRINT D$;"PR#0": PRINT "ATOMIC FLUORESCENCE PROGRAM
ENDED!": PRINT : PRINT " ENTER RUN TO BEGIN AGAIN": END
3220  PRINT D$;"PR#1": PRINT :  PRINT  :  PRINT  : PRINT : PRINT :
PRINT D$;"PR#0": GOTO 3130
3230  REM  ******************
3240  REM  **KEYBOARD INPUT**
3250  REM  ******************
3260  FOR N = 1 TO NE
3270  FOR I = 1 TO R(RN)
3280   PRINT  :  PRINT  "FOR  ELEMENT ";EL$(N);" CONC. ";C(N,RN);"
READING= ";
3290  INPUT EL(N,RN,I)
3300  NEXT
3310  NEXT
3320  FOR N = 1 TO NE
3321  FOR I = 1 TO R(RN)
3322  GOTO 2400
3330  REM  **END KEYBOARD IN**
3340  REM  ******************
3350  REM  *** HEADER PRINT ***
3360  REM  ******************
3370  IF TI$ <  > ""  THEN X =  LEN (TI$):I = 20 - X / 2: PRINT
TAB( I): PRINT  CHR$ (14);TI$; CHR$ (20): PRINT
3380  IF OP$ < > "" THEN  PRINT "OPERATOR  ";OP$;
3390  PRINT  TAB( 41);"POSITION  ELEMENT  CURRENT   PMT"
3400  IF (DA$ < > "") OR (MO$  <  > "")  OR (YR$ < > "") THEN
PRINT "DATE  ";DA$;" ";MO$;" ";YR$;
3410  IF T$ < > "" THEN  PRINT "     TIME  ";T$;
3420   IF  MP$(1)  <  > ""  THEN   PRINT  TAB( 45);MP$(1); TAB(
14);EL$(1); TAB( 23);LC$(1); TAB( 31);PM$(1)
```

```
3030  IF PO$ <  > ""  THEN    PRINT "POWER  ";PO$;: IF MP$(2) = ""
THEN  PRINT
3440    IF  MP$(2)  <    > "" THEN  PRINT   TAB(  45);MP$(2);  TAB(
14);EL$(2); TAB( 23);LC$(2); TAB( 31);PM$(2)
3450  IF CA$ <    > "" THEN  PRINT "CARRIER FLOW  ";CA$;: IF MP$(3)
= "" THEN  PRINT
3460   IF  MP$(3)  <     >  ""  THEN   PRINT  TAB( 45);MP$(3); TAB(
14);EL$(3); TAB( 23);LC$(3); TAB( 31);PM$(3)
3470  IF CO$ <    > "" THEN  PRINT "COOLANT FLOW  ";CO$;: IF MP$(4)
= "" THEN  PRINT
3480    IF  MP$(4) <  > "" THEN   PRINT    TAB(  45);MP$(4);  TAB(
14);EL$(4); TAB( 23);LC$(4); TAB( 31);PM$(4)
3490   IF PU$ <  > "" THEN  PRINT "PUMP SPEED  ";PU$;: IF MP$(5) =
"" THEN  PRINT
3500   IF MP$(5) <  > ""  THEN    PRINT    TAB(  45);MP$(5);  TAB(
14);EL$(5); TAB( 23);LC$(5); TAB( 31);PM$(5)
3510  IF OX$ <  > "" THEN  PRINT "OXIDANT  FLOW  ";OX$;: IF MP$(6)
= "" THEN  PRINT
3520  IF MP$(6) <    >  ""  THEN    PRINT    TAB(  45);MP$(6); TAB(
14);EL$(6); TAB( 23);LC$(6); TAB( 31);PM$(6)
3530   IF  RE$  <     >  "" THEN  PRINT "REDUCTA#^ FLOW  ";RE$;: IF
MP$(7) = "" THEN  PRINT
3540  IF MP$(7) <    >  ""  THEN    PRINT    TAB( 45);MP$(7); TAB(
14);EL$(7); TAB( 23);LC$(7); TAB( 31);PM$(7)
3550    IF  MP$(8) <  > "" THEN   PRINT    TAB(  45);MP$(8);  TAB(
14);EL$(8); TAB( 23);LC$(8); TAB( 31);PM$(8)
3560   IF  MP$(9)  <    >  ""  THEN   PRINT  TAB( 45);MP$(9); TAB(
14);EL$(9); TAB( 23);LC$(9); TAB( 31);PM$(9)
3570  IF MP$(10) <  > ""  THEN    PRINT    TAB(  45);MP$(10); TAB(
14);EL$(10); TAB( 23);LC$(10); TAB( 31);PM$(10)
3580    IF  MP$(11) <  > "" THEN  PRINT   TAB(  45);MP$(11);  TAB(
14);EL$(11); TAB( 23);LC$(11); TAB( 31);PM$(11)
3590  IF MP$(12) <    >  ""  THEN    PRINT   TAB( 45);MP$(12); TAB(
14);EL$(12); TAB( 23);LC$(12); TAB( 31);PM$(12)
3600  IF R1$ <  > "" THEN  PRINT "REMARKS  ";R1$
3610  IF R2$ <  > "" THEN  PRINT "REMARKS  ";R2$
3620  IF R3$ <  > "" THEN  PRINT "REMARKS  ";R3$
3630  IF R4$ <  > "" THEN  PRINT "REMARKS  ";R4$
3640  PRINT : PRINT D$;"PR#O"
3650  RETURN
3660  REM *****************
3670  REM END HEADER PRINT**
3680  REM  ***********************
3690  REM   MENU MODE PRINT
3700  REM  ***********************
3710  HOME
3720   INVERSE  :  PRINT  "SELECT  EXTERNAL PRINTER IN MENU MODE":
PRINT : PRINT "HIT CONTROL RESET TO ESCAPE!": NORMAL
3730  PRINT D$: PRINT D$;"IN#2"
3740  FOR I = 0 TO 71
3750  GET A$(I)
3760  NEXT  3770  FOR I = 72 TO 92
3780  INPUT A$(I)
3790  IF  RIGHT$ (A$(I),6) = "CYCLES" GOTO 3810
3800  NEXT
```

```
3810  PRINT D$;"IN#O"
3820  PRINT D$: PRINT D$;"PR#1"
3030  FOR I = O TO 71
3840  PRINT A$(I);
3850  NEXT : PRINT
3860  FOR I = 72 TO 92
3870  PRINT A$(I)
3880  IF  RIGHT$ (A$(I),6) = "CYCLES" GOTO 3900
3890  NEXT
3900  PRINT D$;"PR#O"
3910  GOTO 3720
3920  REM  ********************
3930  REM   END OF MENU PRINT
3940  REM  ********************
```

PROGRAM OUTPUT SECTION

The following is an example of a printout produced using the option of all data full header.

DETECTION LIMITS PROGRAM EXAMPLE

OPERATOR ALLEN MEIER
DATE 30 JULY 1984 TIME AM
POWER 550 WATTS
CARRIER FLOW 1.3
COOLANT FLOW 12
PUMP SPEED 425
OXIDANT FLOW 0
REDUCTANT FLOW 50
REMARKS THIS AN EXAMPLE OF A PRINTOUT!
REMARKS THE VALUES LISTED HERE ARE ONLY FOR EXAMPLE!

POSITION	ELEMENT	CURRENT	PMT
1	CA	18.2	600 V
2	CU	13.4	650 V
4	K	10.3	850 V
6	ZN	11.1	700 V
12	MG	18.2	600 V

ELEMENT CA RUN=1 REPS.=10 CONC.=0 UG/ML MEAN=1786 STD.DEV.=33 RSD%=1.86
RAW DATA 1777 1767 1787 1776 1877 1776 1787 1787 1756 1775 NET COUNTS= 0
ELEMENT CA RUN=2 REPS.=3 CONC.=10 UG/ML MEAN=5595 STD.DEV.=61 RSD%=1.10
DET. LMT. 174.53 UG/L RAW DATA 5555 5565 5667 NET COUNTS= 3809.16667

ELEMENT CU RUN=1 REPS.=10 CONC.=0 UG/ML MEAN=739 STD.DEV.=369 RSD%=49.9
RAW DATA 1787 606 621 634 585 598 578 668 657 665 NET COUNTS= 0
ELEMENT CU RUN=2 REPS.=3 CONC.=1 UG/ML MEAN=9880 STD.DEV.=6 RSD%=.067
DET. LMT. 80.814 UG/L RAW DATA 9876 9877 9888 NET COUNTS= 9140.43333

ELEMENT K RUN=1 REPS.=10 CONC.=0 UG/ML MEAN=59 STD.DEV.=189 RSD%=316.
RAW DATA 599 0 0 0 0 0 0 0 0 0 NET COUNTS= 0
ELEMENT K RUN=2 REPS.=3 CONC.=.5 UG/ML MEAN=3010 STD.DEV.=9 RSD%=.332
DET. LMT. 64.208 UG/L RAW DATA 3000 3020 3010 NET COUNTS= 2950.1

ELEMENT ZN RUN=1 REPS.=10 CONC.=0 UG/ML MEAN=5 STD.DEV.=4 RSD%=70.2
RAW DATA 0 9 9 0 8 9 0 9 7 7 NET COUNTS= 0
ELEMENT ZN RUN=2 REPS.=3 CONC.=2 UG/ML MEAN=10100 STD.DEV.=100 RSD%=.990
DET. LMT. 1.6155 UG/L RAW DATA 10000 10100 10200 NET COUNTS= 10094.2

ELEMENT MG RUN=1 REPS.=10 CONC.=0 UG/ML MEAN=123 STD.DEV.=309 RSD%=250.
RAW DATA 7 8 8 8 9 90 90 999 9 9 NET COUNTS= 0
ELEMENT MG RUN=2 REPS.=3 CONC.=5 UG/ML MEAN=20066 STD.DEV.=57 RSD%=.287
DET. LMT. 155.15 UG/L RAW DATA 20000 20100 20100 NET COUNTS= 19942.9667