AAFLAME

(VERSION 2.1)

PROGRAMS FOR ATOMIC ABSORPTION AND FLAME EMISSION

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22 July 2005

INTRODUCTION

AAFLAME is a collection of programs for atomic absorption and flame emission analysis. You can correct for curvature and drift. You can calculate original sample concentrations by entering sample and diluted weights. Sample names and weights can be entered and stored for future use. The program works with a Pico ADC-16 data logger. You may also enter absorbances from the keyboard.

This is not a step by step manual. The best way to learn is to try the program. Prompts are displayed where needed.

This program, provides a low cost way of upgrading older atomic absorption spectrometers to modern standards, or better. Many modern instruments do not provide facilities such as drift correction, for example.

PROGRAM OUTLINES

LINEAR is a simple linear program for atomic absorption. You run a standard, a blank and a series of samples. The calculated concentrations are immediately displayed and, at the end of the run, a summary is printed and archived on disk.

DRIFT is a linear program for atomic absorption which provides for drift correction. You run a standard, a blank, a series of samples, the blank again and the standard again. Concentrations without drift correction are displayed during the run. At the end of the run drift corrected calculations are displayed, printed and archived on disk.

Just before the standard is run a second time, the uncorrected results are saved in the file **AADATA.DAT**. At the end of the run the corrected results are saved in the same file.
The same thing happens in **BICURVE** and **ABSTRAY**. In all of these programs you also have the option of entering and storing sample names, sample weight before dilution and total weight after dilution. The names and weights may be stored on keys **F1..F10**, any number key, or any letter key. The weights allow the reporting of concentrations in the original samples. The names and weights may retrieved from the same key.

CURVE is a program for the correction of curvature. I originally published the algorithm used in this program in Analytica Chimica Acta, 107 (1979) 201-209. It is especially useful for flame emission. It also corrects many forms of atomic absorption curvature. Two or three standards and a blank are run. A calibration curve is displayed. A series of samples are run and calculated concentrations are displayed during the run. At the end of the run a summary is printed and archived on disk.

STRAY also corrects curvature. It assumes curvature is caused by non resonant light from the hollow cathode lamp. It is useful for some forms of atomic absorption curvature. Two standards and a blank are run. A calibration curve is displayed. A series of samples are run. The calculated concentrations are displayed during the run. At the end of the run a summary is printed and archived on disk. See "Atomic Spectrometry Programs for the HP 9815A Computing Controller" Report CD2309, J E Patterson, Chemistry Division, DSIR, November 1980 for an explanation of this algorithm. There is also useful information on **CURVE** and an early version of **DRIFT**.

BICURVE combines **CURVE** with **DRIFT**. In other words both curvature and drift are corrected. Two or three standards are run, then a blank, a series of samples, a blank and two or three standards

again. A calibration curve is displayed before the samples are run. The curvature corrected concentrations are displayed during the run. A second calibration curve is displayed after the second set of standards. At the end of the run concentrations corrected for curvature and drift are displayed, printed and archived on disk.

ABSTRAY combines **STRAY** with **DRIFT**. Two standards are run, then a blank and two standards again. A calibration curve is displayed before the samples are run. The curvature corrected concentrations are displayed during the run. A second calibration curve is displayed after the second set of standards. At the end of the run concentrations corrected for curvature and drift are displayed, printed and archived on disk.

In all programs data is stored in **AADATA.DAT**, appended in compact form to a daily file like **93032218.aa**. The file name and heading are appended to **AAFILES.CAT**. This makes it easy to find old data. In the drift programs files like **AALABEL.DF1** or **AALABEL.DAB** are created, where **F1** or **B** were pressed to store sample names and weights. Use **WRITE** to view any of these files.

WRITE is simple editor for correcting headings, names, etc in stored data and generating reports.

PRINT sends a copy of the backup file **AADATA.DAT** to the printer. This file contains a copy of the last set of results.

HELP contains information on program operation. Prompts are also displayed within the programs.

EQUIPMENT

Any IBM compatible computer with a hard drive can be used. You need one serial port for the data logger and one parallel port for a printer. The printer can be of any type as only text is printed.

The data logger is a PICO ADC-16 high resolution data logger produced by PICO Technology.

http://www.picotech.com

You will need to specify the data logger input voltage ranges to suit your AA analog output. Drivers can be written for other systems. Channels 2, 3 and 4 are also logged at the end of the printed report. Two channels can be connected to log lamp current and photomultiplier gain for example.

Data is logged into the same directory where the program is stored. You should periodically move old files to a backup disk or directory.

MAIN MENU

The main menu is shown below. Press a key to run a program. You will also be asked to turn the printer on if it is off.

```
                        <<<<  AA-FLAME 2.1 >>>>

                    Programs for atomic spectrometry
                            By J E Patterson


                    Type a letter to choose a program

            L: LINEAR  - linear atomic absorption
            D: DRIFT   - correction of linear drift
            C: CURVE   - correction of spectral curvature
            S: STRAY   - correction of stray light curvature
            B: BICURVE - curvature with drift correction
            A: ABSTRAY - stray light with drift correction
            W: WRITE   - text editor to view and modify files
            P: PRINT   - print backup file AADATA.DAT
            H: HELP    - help information
            E: EXIT    - exit to DOS

                                NOTICE (31/3/93)
In the drift programs you may, instead of entering the sample
number, just press ENTER.  You will be asked to press a key and then
enter a name.  Sample and dilution weights are entered also.  Press
ENTER to end.  Press SPACEBAR, ENTER and a key to recall sample names.
```

LINEAR

The following shows a typical screen for **LINEAR**. The programs **CURVE** and **STRAY** are similar except that more standards are asked for.

The previous heading may be recalled by pressing the **ENTER** key. The heading may be altered by using **BACKSPACE** and typing new information.

RUN STANDARD or **RUN SAMPLE** means press the **ENTER** key to capture data from the AA. You may alternatively enter a number from the keyboard and then **ENTER**.

```
93032218.16-                        LINEAR                    Press Esc to exit
                              22/03/93  18:16
                              Linear AA program

------------------------------------------------------------------------------
Test samples for AA. Copper 327.4nm.
------------------------------------------------------------------------------
Enter number of readings (e.g. 5) 12  No. Absorbance   %RSD   Concentration

Enter concentration of standard   5    1     0.2300     0.3      2.381E+00
                                       2     0.2200     0.4      2.262E+00
Run standard   .45

Run blank      .03

Run sample .15

Conc sample = 2.262E+00
```

%RSD = ABS(standard deviation/average absorbance*100). This applies to the observed value, not the concentration.

See **DRIFT** for examples of backup, archived and printed files.

DRIFT

The following shows a typical screen for **DRIFT**. The programs **BICURVE** and **ABSTRAY** are similar except that more standards are asked for.

The previous heading may be recalled by pressing the **ENTER** key. The heading may be altered by using **BACKSPACE** and typing new information.

You may, instead of entering the number of samples, just press **ENTER**. You will be asked to press a function key **F1..F10**, a number or a letter. Press a key and enter a name. Press **ENTER** alone to finish.

Press **SPACEBAR**, **ENTER** and then **F1..F10**, a number or a letter to recall stored sample names.

RUN STANDARD or **RUN SAMPLE** means press the **ENTER** key to capture data from the AA. You may alternatively enter a number from the keyboard and then **ENTER**.

Press **ESC** to exit

```
93040316.44-                  Drift Correction           Press Esc to exit
                              03/04/93  16:44
           A program for correcting linear drift in spectral data

-------------------------------------------------------------------------
 BCS 367 and US BSFs  ,   SiO2
-------------------------------------------------------------------------
Enter number of readings (e.g. 5) 12 No.  Absorbance   %RSD   Concentration
                                      1     0.0290      3.5      2.262E+01
Sample names retrieved from F3        2     0.0542      1.4      4.378E+01
                                      3     0.0732      1.1      5.971E+01
Enter concentration of standard  493  4     0.5207      0.3      4.345E+02
                                      5     0.0062      8.4      3.638E+00
Run standard          .5879

Run blank             .0022

Run blank             .0019

Run standard          .5919_
```

If you have a large number of samples you have the option of running all the samples in one long batch with standards at each end or several smaller batches with sample names and weights stored on several keys. In the first case you should run a standard and blank periodically to check that the drift was corrected properly. If not, then you can use **DRIFT** again to manually recorrect the data.

PRINTED SUMMARY

A printed summary from the **DRIFT** run is shown below.

```
------------------------------------------------------------------
93040316.44-
          Linear drift correction with blank,  JEP9208
                          03/04/93  16:44
 BCS 367 and US BSFs  ,   SiO2
Sample names saved on key: F3

Standard Concentration          Absorbance               %RSD
      4.930E+02                   0.5879                  0.3
      0.000E+00                   0.0022                 18.2
      0.000E+00                   0.0019                 39.0
      4.930E+02                   0.5919                  0.3

                                   Dilute    Dilute   Sample     Sample
Sample number   Absorbance  %RSD   solution   weight   weight  concentration
                                    (ppm)      (g)      (g)        (ppm)
BCS 376 O-DEM     0.0290    3.5   2.262E+01   25     8E-002     7.069E+03
US-BFS O-DEM      0.0542    1.4   4.378E+01   24.9   8.06E-002  1.353E+04
BCS 367 K-DEM     0.0732    1.1   5.971E+01   26     8.08E-002  1.921E+04
US BFS K-DEM      0.5207    0.3   4.345E+02   25.3   8.2E-002   1.340E+05
K-DEM BLK         0.0062    8.4   3.638E+00   25     8E-002     1.137E+03

Other logger channels
Channel 2 = 0
Channel 3 =-.4
Channel 4 = 0
```

The data is also saved temporarily in **AADATA.DAT** and is added to **93040316.aa** in a more compact format, as follows. Press P from the main menu to print **AADATA.DAT**.

```
93040316.44-
Linear drift correction with blank,  JEP9208
 BCS 367 and US BSFs  ,   SiO2
F3
 4.930E+02, 0.5879, 0.3
 0.000E+00, 0.0022,18.2
 0.000E+00, 0.0019,39.0
 4.930E+02, 0.5919, 0.3
BCS 376 O-DEM, 0.0290, 3.5, 2.262E+01, 25 , 8E-002 , 7.069E+03
US-BFS O-DEM, 0.0542, 1.4, 4.378E+01, 24.9 , 8.06E-002 , 1.353E+04
BCS 367 K-DEM, 0.0732, 1.1, 5.971E+01, 26 , 8.08E-002 , 1.921E+04
US BFS K-DEM, 0.5207, 0.3, 4.345E+02, 25.3 , 8.2E-002 , 1.340E+05
K-DEM BLK, 0.0062, 8.4, 3.638E+00, 25 , 8E-002 , 1.137E+03
Ch 2 = 0
Ch 3 =-.4
Ch 4 = 0
```

This data can be loaded into a spreadsheet, for further treatment.

HELP

The following information is displayed when **H** is pressed.

```
    The previous heading may be recalled by pressing the ENTER key.
    The heading may be altered by using BACKSPACE and typing new
    information.

    RUN STANDARD or RUN SAMPLE means press the ENTER key to capture
    data.  You may alternatively enter a number from the keyboard and
    then ENTER.

    The current data set is stored temporarily in a file AADATA.DAT.
    This allows data to be retrieved from a drift correction where
    the second run of standards goes wrong.  Data is also archived,
    in compressed form, in a file with a name like 920726.AA, where
    the number is the year, month and day.  A new file is created
    automatically each day.

    A file called AAFILES.CAT accumulates the file date and heading
    from each run, to aid retrieval of old data.

    In the drift programs you may, instead of entering the sample
    number, just press ENTER.  You will be asked to press a key and then
    enter a name.  Sample and dilution weights are entered also.  Press
    ENTER to end.  Press SPACEBAR, ENTER and a key to recall sample names.
Press ESC to exit
```

WRITE

Write is a simple editor which will allow you to alter or correct data files. Adding information to the heading is a typical application. The editor has the same menu structure as **SPECRET** for selecting directories and selecting files to edit. The editor is derived from the **BORLAND Turbo Editor Toolbox** and uses the same **WORDSTAR** commands as many other editors.

When the program is run the following screen is displayed:

```
                    WRITE DATA FILE EDITOR

                         J E Patterson


    This program allows data files to be edited.  For instance,
    you may wish to change the information in the heading.

    The following are the most important commands:

    ARROW KEYS (UP, DOWN, LEFT, RIGHT) - move cursor around file.
    PAGE UP, PAGE DOWN - Move up or down one page, less one line.
    HOME or END - move to beginning or end of line.
    Ctrl and PAGE UP or PAGE DOWN - move to file beginning or end.
    BACKSPACE - delete character to the left of the cursor.
    DEL - delete character under the cursor.
    INS - toggle the insert mode on or off.
    F2 - save the file, then continue edit.
    ESC - option to save the file, if altered, then exit.

Press SPACEBAR to continue or ESC to exit
```

Press the **SPACEBAR**. Enter the disk drive where the spectra are stored, e.g. **D:** and **press RETURN**. If the spectra are stored on the current drive then just press **RETURN**. Use the **ARROW** keys to choose a file or another directory. If a file is chosen and **RETURN** is pressed it will be loaded ready for editing.

KEYBOARD COMMANDS

FUNCTION	KEYS	ALTERNATIVE
Character left	Left arrow	Ctrl S
Character right	Right arrow	Ctrl D
Word left	Ctrl left arrow	Ctrl A
Word right	Ctrl right arrow	Ctrl F
Line up	Up arrow	Ctrl E
line down	Down arrow	Ctrl X
Scroll up	Ctrl W	
Scroll down	Ctrl Z	
Page up	PgUp	Ctrl R
Page down	PgDn	Ctrl C

Beginning of file	Ctrl PgUp	Ctrl Q R
End of file	Ctrl PgDn	Ctrl Q C
Beginning of line	Home	Ctrl Q S
End of line	End	Ctrl Q D
Top of screen	Ctrl Home	Ctrl Q E
Bottom of screen	Ctrl End	Ctrl Q X
Goto line	Ctrl J L	
Goto column	Ctrl J C	
Top of block	Ctrl Q B	
Bottom of block	Ctrl Q K	
Jump to marker 0..9	Ctrl Q 0..Ctrl Q 9	
Set marker 0..9	Ctrl K 0..Ctrl K 9	
Previous cursor position	Ctrl Q P	
New line	Enter	Ctrl M
Insert line	Ctrl N	
Insert control character	Ctrl P	
Tab	Tab	Ctrl I
Delete current character	Del	Ctrl G
Delete character left	Backspace	Ctrl H
Delete word	Ctrl T	
Delete to end of line	Ctrl Q Y	
Delete line	Ctrl Y	
Find pattern	Ctrl Q F	
Find and replace	Ctrl Q A	
Find next	Ctrl L	
Abandon file (save if changed)	Esc	Ctrl K Q
Save and continue edit	F2	Ctrl K S
Save and exit editor	Ctrl K X	
Save to file	Ctrl K N	
Add window	Shift F3	Ctrl O A
Next window	F6	Ctrl O N
Previous window	Shift F6	Ctrl O P
Resize current window	Ctrl O S	
Begin block	F7	Ctrl K B
End block	F8	Ctrl K K
Copy block	Ctrl K C	
Move block	Ctrl K V	
Delete block	Ctrl K Y	
Hide block	Ctrl K H	
Mark current word as block	Ctrl K T	
Read block from file	Ctrl K R	
Write block to file	Ctrl K W	
Toggle insert mode	Ins	Ctrl V
Toggle autoindent mode	Ctrl Q I	

Toggle marker display	Ctrl K M
Change directory	Ctrl J D
Show version	Ctrl J V
Show available memory	Ctrl J R
Set undo limit	Ctrl J E
Set default extension	Ctrl J E
Abort command	Ctrl U
Undo last deletion	Ctrl Q U
Restore line	Ctrl Q L

If you find any errors or require any changes please let me know.

J E Patterson
22 July 2005