Connecting IBM Personal Computers to Agilent SpectrAA Atomic Absorption Spectrometers

Application Note

Atomic Absorption

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Introduction

There are many considerations in selecting PC hardware options for the laboratory. Choosing amongst these options can seem a daunting task to the uninitiated.

For example; often, the base PC consists only of a computer module with keyboard, printer, and RS-232 port. A range of options is then available, such as extra RAM (Random Access Memory); communications ports; an arithmetic co-processor; a floppy/hard disk system versus a dual floppy disk system; monochrome, CGA (Color Graphics Adaptor), EGA (Enhanced Graphics Adaptor) display cards and monitors. However, unlike the somewhat unpredictable needs of many business users, the choice of options for the laboratory, may be more clearcut if some of the following aspects are considered.

RAM is used by the PC to load the program and manipulate data. A PC with less than 512K RAM may not be able to use some of the more sophisticated software programs. In general, 640K of RAM is recommended for the processing of large arrays of analytical data, or when using memory-resident programs such as SideKick. When considering buying more memory, it should be noted that not all programs can address more than 640K of RAM.

An arithmetic co-processor (a retrofittable option) may provide additional speed when using software programs which perform a significant amount of arithmetic calculation. (for example, Lotus 1-2-3). It is best to check a program's documentation to see if specific reference is made to being able to use this facility.

Where frequent storage of analytical data is required or, where other commercial programs such as Lotus 1-2-3 are used, a hard disk can provide significant benefits. These benefits are not only in storage capacity, but also in speed, ease of loading other programs, and ease of operation for infrequent PC users.

The use of an EGA card with compatible video monitor is also desirable for laboratory use. Most PC programs make good use of color to simplify program operation. The EGA's maximum graphics resolution of 640 × 350 pixels, with 16 colors, as compared with the CGA's maximum of 320 × 200 pixels, with 4 colors (640 × 200 pixels,

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monochrome), better exploit the capabilities of modern software packages. In the case of the popular Lotus 1-2-3 package, this means greater text clarity and graph resolution in the presentation of analytical data.

Utility Programs for Laboratory PCs

Once the laboratory PC user has selected amongst the various PC hardware options, the next step is to select software to put the PC to use. This selection also involves a myriad of options. In order to make this task easier, here is a list of utility software that we have found useful:

Lotus 1-2-3	Spreadsheet, database
SideKick	Desktop organizer
Xtree/Xtree Professional	File/directory management
ARC	File archiving
The Complete PC Tutorial	Introduction to PCs

These programs increase both PC productivity and the acceptance of PCs by personnel unfamiliar with their use.

Lotus 1-2-3 (Release 2) is a widely used spreadsheet/database package. It is available from Lotus Development Corp. or most PC suppliers. An important requirement for such a package in laboratory use is the facility for versatile graphics presentations. Unlike a number of its contemporaries, Lotus has powerful and easy to use graphics features and interfaces to a wide range of printers and plotters for publication quality printouts. Some AA applications of Lotus 1-2-3 are discussed later.

SideKick, (available from Borland International or most PC suppliers), is a desktop organizer with a number of utilities in pop-up windows. The utilities include a simple Wordstar-like ASCII text editor (Notepad), as well as a full function calculator, calendar, appointment datebook, phone directory etc. The Notepad is useful for viewing and editing instrument results and reports stored in ASCII text files, as well as producing DOS Batch programs to automate PC operation. Being memory-resident, it can be used while other programs are loaded.

Xtree, or the more comprehensuve Xtree Professional, (from Executive Systems Inc. or most PC suppliers), are popular PC utility programs which provide many useful commands for copying, viewing, deleting and maintaining the many data files which invariably end up being stored on disk in laboratory applications. They also provide an excellent overview of directories, programs and data files on hard or floppy disks.

ARC is an archive program, which can be downloaded from most PC bulletin boards through a modem connected to the PC. It can be used to archive programs, analytical data and reports on disk in compressed format. This program provides two main advantages. Firstly, multiple files can be stored under one filename to simplify housekeeping. Secondly, large savings in disk space are possible (typically 75% to 85% compression), since many analytical reports are stored in text format. For example, Report Manager data and reports for a particular month, department or analysis type could be archived together allowing (at say 80% compression) up to 1.8 Megabytes of data to be archived on a single 360 Kilobyte floppy disk.
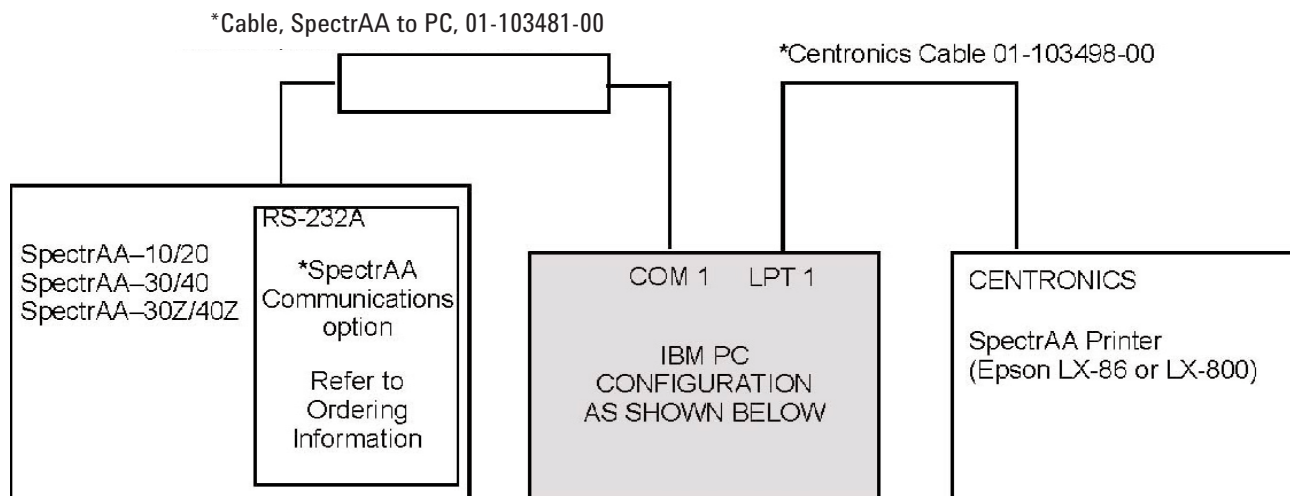
The Complete PC Tutorial, by Intouch Computing, is a tutorial program with simple explanations of DOS commands, BASIC and assembly programming and examples of their application. Being memory-resident, it prompts the operator to use examples of each command, simplifying the learning process. PC operation is covered from beginner to potential programmer and even experienced users can learn of hidden features and shortcuts. This allows beginners to become familiar with the PC without tying up the resources of other PC users in the laboratory. In view of its benefits for many laboratories, this program is available through Agilent (p/n 85-100705-00 for 5.25″ disk format, or p/n 85-100724-00 for 3.5″ disk format).

Collecting AA Data on a PC Using the SpectrAA/PC Report Manager

The SpectrAA/PC Report Manager is a software package providing a variety of new capabilities for generating customized reports from Agilent SpectrAA series AA spectrometers. The package is compatible with Agilent SpectrAA-10/20, 30/40 or 30/40 Zeeman series Atomic Absorption spectrometers for flame, furnace and hydride analysis.

Two options are available to transfer data from the spectrometer to the computer:

1. The SpectrAA Communications Interface, which includes bi-directional RS-232C, IEEE and GPIO protocols (for SpectrAA 30/40/30Z/40Z models, p/n 00-100372-00, for SpectrAA-10/20 models, p/n 00-100335-00 [240 VAC], p/n 00-100335-01 [115 VAC] or p/n 00-100335-02 [220 VAC]). An RS-232 cable (p/n 01-103481-00) is required to connect the PC to the interface (this cable includes a 9/25 pin adapter for both types of RS-232 connectors used on PCs). or

2. A low cost SpectrAA Parallel/Serial Convertor Interface (for SpectrAA 10/20/30/40/30Z/40Z models, p/n 01-103606-00 [230/240 VAC], p/n 01-103607-00 [115 VAC], or p/n 01-103618-00 [220 VAC]). This interface connects to the SpectrAA printer output using the existing SpectrAA printer cable (p/n 01-103078-00) and includes an RS-232 cable with 9/25 pin adapter for connection to PCs with either 9 or 25 pin RS-232 ports.

*Cable, SpectrAA to PC, 01-103481-00   *Centronics Cable 01-103498-00

SpectrAA–10/20 SpectrAA–30/40 SpectrAA–30Z/40Z	RS-232A *SpectrAA Communications option Refer to Ordering Information

COM 1   LPT 1 IBM PC CONFIGURATION AS SHOWN BELOW

CENTRONICS SpectrAA Printer (Epson LX-86 or LX-800)

*Items must be ordered separately

IBM PC Configurations

The SpectrAA/PC Report Manager program is certified for use only with the following configurations:

IBM PC/XT configurations

An IBM PC/XT fitted with either CGA or EGA color monitor and graphics card, a minimum of 512K RAM memory, 360K 5.25" floppy disk drive, one other floppy or hard disk drive, standard XT keyboard, DOS 3.1 and AST SixPakPlus card (from AST Research Inc.) with clock/calendar and serial/parallel port facilities. A hard disk drive is recommended but is not essential.

IBM PC/AT configurations

An IBM PC/AT (6 or 8 MHz version) fitted with IBM EGA color monitor and graphics card, a minimum of 512K RAM memory, 1.2MB 5.25" floppy disk drive, an IBM 20MB or 30MB hard disk drive, IBM AT keyboard, IBM serial/parallel card and DOS 3.1 (6 MHz version) or DOS 3.2 (8 MHz version).
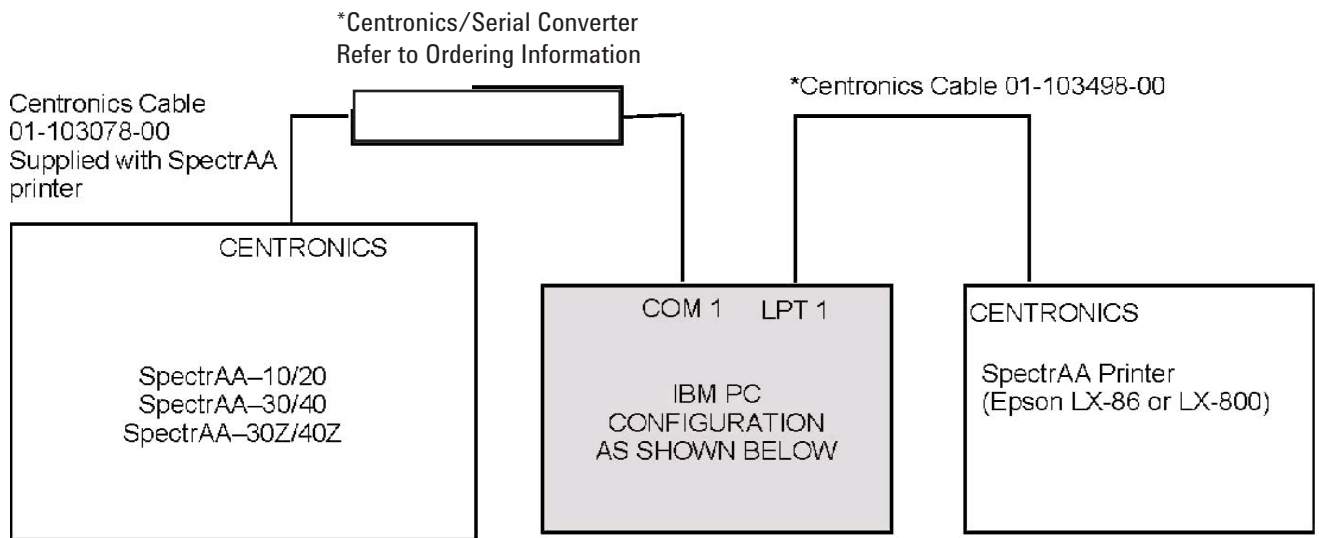
IBM PS/2 Model 30 configurations

An IBM Model 30 fitted with either IBM color display monitor 8512 or 8513, or BasicTime/Qubie EGA card, and monitor, a 720K 3.5" floppy disk drive, one other 3.5" floppy drive or 20MB hard disk drive, Model 30 keyboard, IBM serial/parallel ports and DOS 3.3 software.

IBM PS/2 Model 50/60 configurations

An IBM Model 50 or 60 fitted with either IBM color display monitor 8512 or 8513, a 1.44MB 3.5" floppy drive, 20MB hard disk drive, Model 50/60 keyboard, IBM serial/parallel ports and DOS 3.3 software.

Figure 1.   SpectrAA interconnection (SpectrAA Communications option).

*Centronics/Serial Converter
Refer to Ordering Information

*Centronics Cable 01-103498-00

Centronics Cable
01-103078-00
Supplied with SpectrAA
printer

CENTRONICS

SpectrAA–10/20
SpectrAA–30/40
SpectrAA–30Z/40Z

COM 1   LPT 1

IBM PC
CONFIGURATION
AS SHOWN BELOW

CENTRONICS

SpectrAA Printer
(Epson LX-86 or LX-800)

*Items must be ordered separately

IBM PC Configurations

The SpectrAA/PC Report Manager program is certified for use only with the following configurations:

IBM PC/XT configurations

An IBM PC/XT fitted with either CGA or EGA color monitor and graphics card, a minimum of 512K RAM memory, 360K 5.25″ floppy disk drive, one other floppy or hard disk drive, standard XT keyboard, DOS 3.1 and AST SixPakPlus card (from AST Research Inc.) with clock/calendar and serial/parallel port facilities. A hard disk drive is recommended but is not essential.

IBM PC/AT configurations

An IBM PC/AT (6 or 8 MHz version) fitted with IBM EGA color monitor and graphics card, a minimum of 512K RAM memory, 1.2MB 5.25″ floppy disk drive, an IBM 20MB or 30MB hard disk drive, IBM AT keyboard, IBM serial/parallel card and DOS 3.1 (6 MHz version) or DOS 3.2 (8 MHz version).

IBM PS/2 Model 30 configurations

An IBM Model 30 fitted with either IBM color display monitor 8512 or 8513, or BasicTime/Qubie EGA card,and monitor, a 720K 3.5″ floppy disk drive, one other 3.5″ floppy drive or 20MB hard disk drive, Model 30 keyboard, IBM serial/parallel ports and DOS 3.3 software.

IBM PS/2 Model 50/60 configurations

An IBM Model 50 or 60 fitted with either IBM color display monitor 8512 or 8513, a 1.44MB 3.5″ floppy drive, 20MB hard disk drive, Model 50/60 keyboard, IBM serial/parallel ports and DOS 3.3 software.

Figure 2.   SpectrAA interconnection (Centronics/Serial Converter).

Both interfaces allow data to be read into the PC at speeds up to 9600 baud through the RS-232C port (standard on most PC versions).

For hard copy printouts from the PC, the standard SpectrAA printer (Epson LX-86 or LX-800) can be connected to the PC parallel port using a PC Centronics cable (p/n 01-103498-00).

The SpectrAA/PC Report Manager software operates with IBM PC/XTs, PC/ATs, and PS/2 Models 30, 50 and 60. For PC XT/AT versions, the Report Manager is provided on 5.25" disk format (p/n 85-100700-00) and for PS/2 Models 30, 50 and 60, a 3.5" disk format is provided (p/n 85-100728-00).

PC hardware configurations and system connection details are outlined in Figures 1 and 2. Although not required for use with the Report Manager program, a PC fitted with hard disk and EGA graphics is recommended (see PC hardware options mentioned previously).

SpectrAA/PC Report Manager Facilities

Through close liaison with AA spectroscopy users, the Report Manager program has been designed to accommodate the requirements of both routine and research laboratories. Key facilities include the transfer of AA data to a PC during or after analysis, flexible program customization and automation facilities, report headers and footers, extended sample labels, weight/volume correction, Lab Note storage and integration of flame, furnace and hydride reports providing a choice of over 2000 report formats for industrial QA through to research applications.

The following discusses the capabilities of the Report Manager program and outlines various data processing applications in the AA laboratory of today using Lotus 1-2-3.

Ease of Use

Special attention has been paid to providing an easy to use, yet flexible range of facilities for a variety of laboratory requirements. Simple softkey menus and 'Fill in the Form' parameter tables make operation easy for multiple users. Each user can tailor the program to their own needs and store their report selections under individual batch names rather than entering new parameters each time the program is used. On a day to day basis, the operator can quickly recall the desired setup for each analysis from a catalog window.

For occasional users, context sensitive HELP information is available within the program in pop-up windows. All program text can be modified to the users own requirements if needed. For example, information can be easily converted to

local language using a simple text editor such as Borland SideKick (see Figures 3a and 3b).

```
                    Operator : J. Hacker
                        Date : 09/03/88

             Batch Filename : EFFLUENT
                 Auto Report : Yes
_____

_____

               Report Format : Multi-element Conc only
               Data Reported : Sample Label Match
               Report Output : File

                 Lines/Page :  66
           Characters/Line :  80

           Delete Raw Data : No

               Sample Labels : Yes
         Sample Correction : Weight & volume correction
         Include Lab Notes : No

           Create .DIF File : No
           Create .PRN File : Yes
                                        F1 Help
 1 Edit      2 Create    3 Sample    4 Weight    5 Volume    9 Return
   Page        Report      Labels      Correction  Correction
```

Figure 3a.   REPORT FORMAT page.

```
                    Benutzer : J. Hacker
                        Datum : 09/03/88

             Batch Filename : EFFLUENT
          Automatischer Rapport : Ja
_____

_____

               Rapport Format : Multielement nur Konzentration
           Daten Rapportiert : Muster Namen Auswahl
                 Rapport nach : File

                 Linien/Seite :  66
               Zeichen/Linie :  80

           Rohdaten Lschen : Nein

                 Muster Namen : Ja
         Muster Korrektion : Gewichts & volumen Korrektion
               Labor Notizen : Nein

           DIF File erstellen : Nein
           PRN File erstellen : Ja
                                        F1 Hilfe
 1 Seite     2 Rapport   3 Muster    4 Gewichts  5 Volumen   9 Zurck
   Editieren   Erstellen   Namen       Korrektion  Korrektion
```

Figure 3b.   REPORT FORMAT page after conversion to German using Borland SideKick.

Collection of AA Data During or After Analysis

Of special convenience to many laboratories is the facility to transfer AA data after analysis. For those cases where the PC is used for other laboratory tasks, this avoids delaying analysis until the PC is available. Alternatively, data can be transferred during analysis or downloaded from data files archived with the SpectrAA Utility program.

The Report Manager package also includes an "Edit Results" utility for the SpectrAA. For example if spurious readings occur during an overnight furnace run, both samples and standards can be checked and edited at the SpectrAA, and concentration values, statistics and calibration graph recalculated before sending the results to the PC.

All analytical data available from the SpectrAA, including instrument parameters, element notes, individual blanks, standard and sample readings with mean and %RSD values, and SpectrAA graphics can be transferred to the PC for use by the Report Manager program.

Flexible Report Options

Once the SpectrAA data is collected at the PC, the Report Manager program can be used to quickly generate any number of a wide variety of reports at any time for either immediate printout, storage on disk (in ASCII text format) or conversion to Lotus PRN or DIF formats. For example, a 16 element multielement report for 67 samples can be generated from stored SpectrAA data and archived on hard disk in less than 90 seconds using an IBM PC/AT. Since reports can be generated off-line from the SpectrAA, this allows the instrument to handle an increased sample analysis workload.

Other timesaving options include entry of sample labels, weight and volume correction and report headers and footers before or after analysis for complete analytical records. Flame, furnace and hydride results can also be integrated in a single report (refer Figure 4). Sequential or multielement reports can be tailored to provide as much or as little detail as required through a wide range of options.

```
Washings from treatment vats #5 and #11, analyzed on 16th December.

Equipment used:   Varian SpectrAA 20 AA Spectrometer, Ser. No. 807423
Combined report:  Flame, furnace and hydride analysis, 12 elements.
```

	Cu ug/mL	Fe ug/mL	Al ug/mL	Ni ug/L	Fe ug/L	Mo ug/mL	Li ug/mL	As ug/L	Hg ug/L	Zn ug/mL	Co ug/mL	Ba ug/mL
BLANK	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.0	0.0	0.0	0.00	0.00
STANDARD 1				5.00			1.00	4.0	5.0		5.00	10.00
STANDARD 2					2.00	5.00	2.00			20.0		
STANDARD 3				15.00	4.00		3.00					30.00
STANDARD 4					8.00	20.00				40.0	20.00	
STANDARD 5				25.00		40.00					50.00	50.00
ADDITION 1	1.00	1.00	10.0									
ADDITION 2	2.00	3.00	20.0									
Effluent Vat 5, #1	0.89	1.09	10.1					3.6	2.2	10.2	12.26	10.30
Effluent Vat 5, #2	2.16	2.33	19.0					1.2	3.2	38.5	18.28	40.50
Effluent Vat 5, #3	2.78	3.74	17.4					1.3	1.3	36.5	28.22	38.75
Effluent Vat 5, #4	1.22	1.28	7.6					2.9	1.9	39.8	15.41	46.42
Top Standard	2.01	2.98	20.2					4.0	5.1	40.2	49.88	49.92
Effluent Vat 11, #1				5.15	1.14	2.22	1.05	0.2	0.5	19.8	2.22	21.03
Effluent Vat 11, #2				16.23	8.27	18.28	2.37	3.2	1.1	36.6	8.83	34.05
Effluent Vat 11, #3				21.87	3.76	28.22	3.07	1.1	2.3	40.5	29.32	33.87
Effluent Vat 11, #4				24.64	4.25	35.44	2.01	1.9	1.7	15.4	35.44	44.64
Top Standard				24.87	8.03	39.66	3.03	3.9	5.0	40.1	49.84	49.87

```
Analyst: J Hacker, Production Lab.

Analysts Comments:
Nickel, Cobalt and Molybdenum levels in Vat #11 require investigation ASAP...
```

Figure 4.   Combined flame, furnace and hydride report with header, footer and extended sample labels.

Sample Label Matching Provides a New Capability

The sample label match facility lets the analyst pick specific samples, standards, and QC check samples from a particular analytical run to generate separate reports or exclude unwanted results. In conjunction with this facility, up to 20 alphanumeric characters can be used for each sample label, allowing each sample to be identified with its batch id in the final report.

For example, in an EPA application a QC check sample or standard may be analyzed after every few samples. Using the sample label match facility, the Report Manager can then generate multiple reports, individual reports for specific batch, or sample data only as well as a separate report containing check sample or standard data only. All reports can also be converted to Lotus PRN format for graphical display of data trends etc. (refer Figures 5 a, b and c).

```
Brass analysis:    Batch 090288

NBS Standard material measured after every five sample



Weight correction applied.

                          Cu        Zn
                          PPM       PPM

NBS Standard #1          2.08      0.91
Brass Sample #1          1.31      0.77
Brass Sample #2          1.99      0.93
Brass Sample #3          2.07      0.97
Brass Sample #4          1.97      0.94
NBS Standard #1          2.10      0.92
Brass Sample #5          1.99      0.95
Brass Sample #6          2.00      0.94
Brass Sample #7          2.14      1.02
Brass Sample #8          2.19      1.04
Brass Sample #9          2.13      1.02
NBS Standard #1          2.08      0.91
       Sample #10        2.32      1.11
          #11            2.28      1.07
                         2.22      1.11
```

Figure 5a.   Multielement brass report listing all samples,including NBS check sample measured every 5 samples.

```
Weight correction applied.

                          Cu        Zn
                          PPM       PPM

Brass Sample #1          1.31      0.77
Brass Sample #2          1.99      0.93
Brass Sample #3          2.07      0.97
Brass Sample #4          1.97      0.94
Brass Sample #5          1.99      0.95
Brass Sample #6          2.00      0.94
Brass Sample #7          2.14      1.02
Brass Sample #8          2.19      1.04
Brass Sample #9          2.13      1.02
Brass Sample #10         2.32      1.11
       le #11            2.28      1.07
                         2.22      1.11
                         0.96
```

Figure 5b.   Sample label match used on above report to print sample data without NBS standards.

```
Weight correction applied.

                          Cu        Zn
                          PPM       PPM

NBS Standard #1          2.08      0.91
NBS Standard #1          2.10      0.92
NBS Standard #1          2.08      0.91
NBS Standard #1          2.09      0.91
NBS Standard #1          2.08      0.92
NBS Standard #1          2.09      0.90
      Standard #1        2.07      0.92
                         2.08      0.91
                         2.08      0.91
```

Figure 5c.   Sample label match used to extract NBS check sample data only from Figure 5a. Data could then be used for trend analysis within Lotus 1-2-3.

Lab Notes

In addition to entry of header and footer information for each report, the Lab Notes facility stores up to 5 screen pages of laboratory notes. Notes can be entered for each type of analysis, allowing the analyst to document sample preparation details, operator notes, method bibliographies, quality control requirements etc. rather than include separate notes under each element (Figures 6 and 7 show typical applications). Lab Notes can also be included in final reports if required.

```
                    Operator : J. Roberts
                        Date : 09/03/88

                Batch Filename : E62
                  Auto Report : Yes


         Include Header/Footer : Both header and footer
Report Header :

Washings from treatment vats #5 and #11, analyzed on 16th December.

Equipment used:   Varian SpectrAA 20 AA Spectrometer, Ser. No. 807423
Combined report:  Flame, furnace and hydride analysis, 12 elements.

Report Footer :
Analyst's Comments:              Analyst: J Hacker, Production Lab.
Cobalt levels in Vat #5 fluctuating excessively - monitoring required.
Nickel, Cobalt and Molybdenum levels in Vat #11 require investigation ASAP...



                                         F1 Help
   1 Edit      2 Collect    3 Format    4 Configure  5 Lab      9 Return
   Page         Data        Report       RS-232      Notes
```

Figure 6.   Entry of header and footer information enables customized reports.

```
                            NOTES                        Page 1
          These note pages can be used to store and display sample preparation
          and other analytical details as well as extra help information.
                                          Notes Filename :EFFLUENT

Cadmium in Plant Effluent           Page 1 - sample preparation
Prepared by F. Jones.               Page 2 - analytical conditions
                                    Page 3 - legal discharge limits
CADMIUM in Plant Effluent           Page 4 - stock ordering notes
                                    Page 5 - bibliography

Sample Preparation:
-------------------
a) Filter 100 ml through a Whatman no. 1 filter paper.
b) Transfer part to a 25 ml test tube.
c) Place the test tube in the Varian PSC-56 Sample Changer.
d) Retain the rest of the filtered sample for further tests.

   Samples must be analysed within 24 hours of receipt.


PgUp Previous Page               F1 Help
PgDn Next Page                   Esc Exit Notes Editor
```

Figure 7.   Lab notes facility provides up to 5 pages for operator entered notes.

Report Manager Program Customization

The Report Manager program has been designed to provide maximum flexibility within the program for the majority of applications. However, a wide range of command line options have additionally been provided to allow program customization through DOS BAT programs. These command line options provide external control to select specific data directories, batch filenames, report options, power-up modes, automatic exit to DOS. To illustrate these facilities, a number of example BAT programs are included.

One application for program customization could be automatic data collection and the generation of an AA report using the Report Manager program, followed by Lotus 1-2-3 calculations, without operator intervention. Using the example BAT program supplied, this can be automated through a single command.

Another customized application could be to enter sample data from other analytical instruments (for example, titration and dry weight results, quantitative UV-Vis/ICP/GC/LC data etc.) into the raw data file for inclusion in a Report Manager multielement report with weight/volume correction and PRN/DIF file conversion. Figure 8 shows an example program written in IBM BASIC language to add data from other analytical techniques directly into the Report Manager raw data file.

Data Transfer to Other Laboratory Computers

All Report Manager data can be stored on disk in ASCII text format. The AA data is then as transportable as a PC floppy disk and can be used by other commercial software packages for word processing and desktop publishing applications or transferred between laboratories for round-robin applications.

PC communications software can also be used to transfer AA data to laboratory mainframe computers. This can be done via a modem and phone line or direct connection to the PC. PC Kermit is a widely available public domain PC communications program which can be used for such transfers.

Customization Using Lotus 1-2-3 (Release 2)

The widespread availability and popularity of Lotus 1-2-3 in the chemical laboratory makes it an ideal choice to enhance and customize reports generated automatically by the SpectrAA/PC system.

Lotus can directly import PRN and DIF files created by the Report Manager program into a worksheet. PRN files are special text files which can be directly loaded into Lotus with the Lotus File Import Numbers command. DIF files (Data Interchange Format) are compatible with a range of commercial spreadsheet and database programs.

```
1000 REM BASICA program to add UV-VIS data to Report Manager data files
1010 CLS:GOSUB 1600:  REM  Clear screen and display program information
1050 DIM SAMPLE$(100), CONC(100):  REM  Set arrays for sample labels & data
1060 LF$=CHR$(13)+CHR$(10):        REM  LF$ is a string to print a new line
1100 REM  Enter directory, filename and sample details, lines 1105 to 1140
1105 INPUT "Select desired Report Manager directory  (e.g. C:\DATA.AA) ";DD$
1110 INPUT "Enter a BATCH filename for storage (8 characters) ";F$
1120 DF$=DD$+"\"+F$+".RAW":        REM  Set path/filename for data storage
1130 INPUT "Enter total number of samples (1 to 67) ";MAXSAMPLES
1140 INPUT "Enter CONCENTRATION UNITS (up to 5 characters) ";UNITS$:PRINT
1200 REM  Entry of CONC values for each sample, lines 1210 to 1240
1210 FOR SAMPLE = 1 TO MAXSAMPLES
1220 IF SAMPLE<10 THEN SAMPLE$(SAMPLE)="SAMPLE "+STR$(SAMPLE)+"  ":GOTO 1230
1225 SAMPLE$(SAMPLE)="SAMPLE "+RIGHT$(STR$(SAMPLE),2)+"  "
1230 PRINT "Enter concentration for ";SAMPLE$(SAMPLE);:INPUT CONC(SAMPLE)
1240 NEXT SAMPLE
1300 REM  Stores data on disk in the required format, lines 1310 to 1400
1310 OPEN DF$ FOR APPEND AS 3
1320 PRINT #3,LF$
1330 PRINT #3,SPACE$(8);"PROGRAM 99   UV DATA";LF$:  REM 'UV' is column title
1350 PRINT #3,"SAMPLE          CONC"
1360 PRINT #3,"              "+UNITS$;LF$
1370 FOR SAMPLE = 1 TO MAXSAMPLES
1380 PRINT #3,SAMPLE$(SAMPLE);
1385 PRINT #3,USING "####.##";CONC(SAMPLE):  REM  ####.## sets data format
1390 NEXT SAMPLE
1395 PRINT #3,LF$
1400 CLOSE #3
1500 PRINT:PRINT "Data Directory used for storage:  ";DD$
1510 PRINT "UV Data has been added to BATCH file:  ";F$:PRINT
1520 SYSTEM:  REM exit to DOS
1600 REM   Display program information, lines 1610 to 1690
1610 PRINT "EXAMPLE UV-VIS DATA ENTRY PROGRAM FOR SPECTRAA/PC REPORT MANAGER
1620 PRINT:PRINT "This program appends UV-Vis data to an existing Report ";
1625 PRINT "Manager raw data file."
1630 PRINT:PRINT "If the raw data file does not exist, it will be created.  AA d
ata can then be ";
1635 PRINT "added by entering the new BATCH filename at the Report Manager Heade
r/Footer"
1640 PRINT "page and selecting Collect Data mode.":PRINT
1690 RETURN
```

Figure 8.   An example Basic program to incorporate data from other analytical techniques into a Report Manager report.

By using different areas of the Lotus worksheet the data can be manipulated, acted upon and analyzed for a wide variety of customized applications. For example, if a particular laboratory uses a special format to report analytical results to its customers, that form can most likely be duplicated using a Lotus template. The data from a Report Manager PRN file can be incorporated into this worksheet along with results from other analyses e.g. Titration, ICP, GC, LC, UV results etc. to form a complete analytical report for each sample, in a customized format.

A recent customer request illustrates a typical application of the above. For a brass coating analysis, a customized report was required to list copper and zinc concentrations in ppm units as well as % copper and g/kg coating for each sample. The mean % copper and g/kg values for all samples was also required. By loading a copper/zinc multielement PRN file into a Lotus worksheet, it is a simple matter to add a formula in a column beside the ppm data to calculate % copper. Another column can be added to calculate g/kg coating using the nominal weight (samples can be weight corrected using the Report Manager program). Finally, the average of both columns can be calculated using the Lotus @AVG command.

The ease with which Lotus accomplishes organization and manipulation of data is greatly enhanced through the use of macros. Macros are short programs which duplicate the normal keystroke operations necessary to manipulate the data and generate the final report within Lotus. They are called up by a double keystroke command. (That is hold the Alt key down and press a letter key A to Z corresponding to a letter label given to each macro.) This then automatically executes all the keystrokes and commands contained in the macro. An example of a short macro which automatically imports data from a Report Manager PRN file using an Alt-D command is shown in Figure 9.

```
            Y        Z       AA      AB      AC      AD      AE      AF      AG
   1    The following is a Lotus macro program, executed by pressing ALT D.
   2
   3    To create, type in the macro program listing below.  Then position the
   4    cursor at cell AA10 and select the / R)ange N)ame C)reate commands.
   5    Enter the name as \D and the range as AA10.
   6
   7
   8    Macro Label    Macro Program           Program Comments
   9
  10    \D             {HOME}                  Set cursor to top of worksheet
  11                   /FD                     Enter F)ile D)irectory commands
  12                   C:\DATA.AA~             Enter data directory
  13                   /FIN                    Enter F)ile I)mport N)umbers commands
  14                   EFFLUENT.PRN~           Load EFFLUENT.PRN file
  15
  16
  17
  18
  19
  20
  09/03/88   15:06
```

Figure 9.   An example Lotus 1-2-3 macro program to automatically load a Report Manager report into a worksheet.

Macros can be used to completely automate arithmetic calculations and graphical plots of sample data.

Two such macro examples are included with the Report Manager program. One shows how to plot a barchart of the total metal content of multielement samples. Another provides a QA trend analysis plot with computation of mean batch concentration and testing of sample concentration against user entered upper and lower limits (Figures 10 and 11). Using these macros, the only keystroke necessary to complete an entire analysis of data is an Alt-D command (That is, type D while holding the Alt key down).

Two special facilities in Lotus allow automation to be taken much further. Firstly, if a macro is be defined as an AUTOEXE-CUTE macro, it will execute automatically when the Lotus worksheet is loaded. Secondly, if the worksheet containing macros is saved under the filename AUTO123.WK1 in the default Lotus directory, the worksheet will be loaded and executed automatically whenever Lotus is loaded from DOS.

```
                    A              B         C         D         E         F         G
 1   SpectrAA/PC Report Manager filename SEQTREND.PRN
 2   from disk directory                C:\DATA.AA
 3                   Upper Conc Limit       30.5
 4                   Lower Conc Limit       2.5
 5
 6   Press ALT D to plot the above file or ALT X to exit
 7
 8   ACME Analytical Laboratory: Copper analysis
 9
10           PROGRAM 2     Cu IN EFFLUENT
11
12   SAMPLE              CONC          Range    Upper    Lower    Mean
13                       PPM           Test     Conc     Conc     Conc
14
15   Cu batch #12/1      22.5                   30.5     2.5    15.832
16   Cu batch #12/2       9.8                   30.5     2.5    15.832
17   Cu batch #12/3       7                     30.5     2.5    15.832
18   Cu batch #12/4      33.4          Out      30.5     2.5    15.832
19   Cu batch #12/5       7.9                   30.5     2.5    15.832
20   Cu batch #12/6      30.6          Out      30.5     2.5    15.832
09/03/88   15:22
```

Figure 10.   The Report Manager "Auto Trend Analysis" macro in operation, showing range testing against user-entered upper/lower limits.
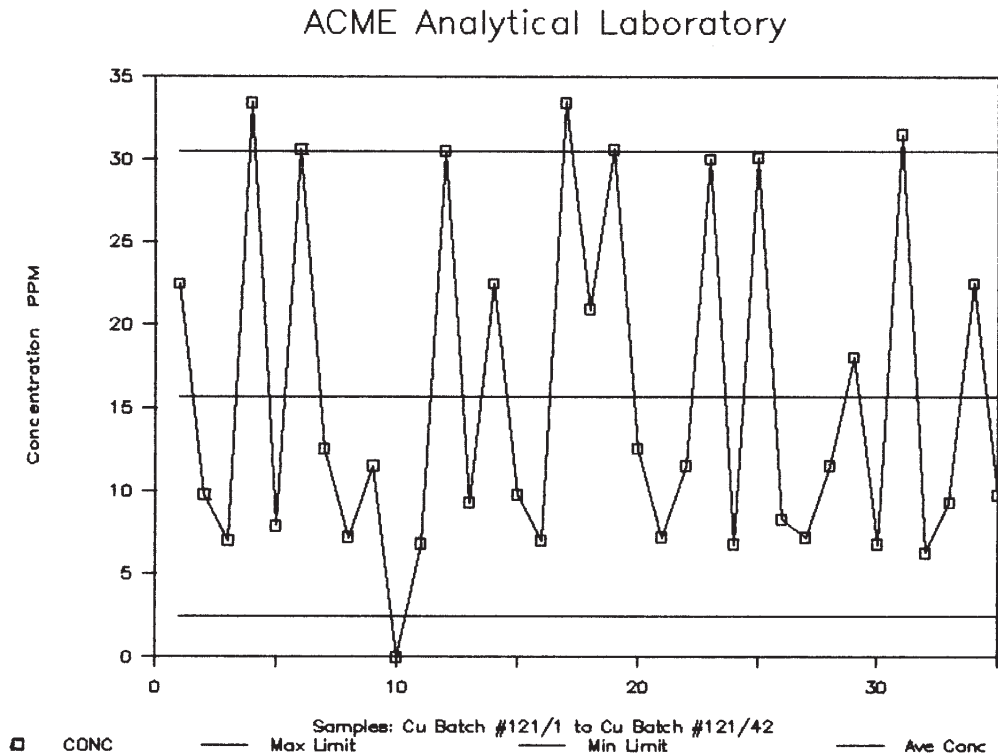

Figure 11.   The Report Manager "Auto Trend Analysis" macro provides graphical plot with display of mean batch concentration and range test limits.

Since this may inconvenience other Lotus users of the laboratory PC, a simple DOS BAT program can easily be used to rename the desired worksheet file before loading Lotus, and rename it to its original filename after exiting (example DOS BAT programs are included with the Report Manager program illustrating these commands). Using this approach, entire Lotus calculations can be performed automatically, without operator intervention or operator knowledge of Lotus, by using a single command from DOS.

Additional capabilities are available using the Lotus 12-3 database facilities. Sample data from individual batches can be added to a database on disk for long term records etc. For example, fields can be added to include date of analysis to allow extraction of all copper results for QC check samples in a specific month. Analytical data can be recalled and sorted in order of increasing or decreasing sample concentration or sample ID. Results within or outside a concentration window can be extracted for further calculations. For more extensive database applications, data can be translated for use with other PC database packages such as Symphony or DBASE III+.

Other Lotus facilities of use in manipulating analytical data include statistics and mathematical functions, frequency distribution and matrix calculations, and multiple regression analysis. For example, one use of the regression facilities could be to apply an alternative calibration algorithm (least squares) to analytical data.

Conclusion

The Agilent SpectrAA/PC Report Manager program is capable of providing increased laboratory productivity through customized reports, transportable data and compatibility with other commercial PC software packages.

The combination of the Report Manager package with Lotus 1-2-3 further enables the analyst to perform a wide range of arithmetic calculations and data analysis, providing new opportunities for laboratories to generate reports to their own specific requirements.

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