

# Transfer and Manipulation of Atomic Absorption Data Using An IBM PC/AT LOTUS 1-2-3 Software and Agilent SpectrAA-40 Spectrometer

## Application Note

Atomic Absorption

### Authors

John Douglass  
Sig Skujins

### Introduction

The ready availability of personal computers has stimulated their use for the collection of analytical data in many laboratories. Once the data has been acquired (off-line or on-line) it can be conveniently archived, manipulated and incorporated into specifically tailored reports.

This paper describes the transfer of analytical data from a SpectrAA Series Atomic Absorption Spectrometer to an IBM PC/AT personal computer, and illustrates how transferred data may be manipulated and reported with the use of commercially available software such as the Lotus 1-2-3.



**Agilent Technologies**

## Experimental

An Agilent SpectrAA 40P AA Spectrometer fitted with the optional Communications Interface (p/n 00-100372-00) was connected to an IBM PC/AT Personal Computer via a RS-232C cable (p/n 01-103481-00).

The IBM PC/AT used was equipped with 512K RAM, 1.2 MB floppy disk drive, 20 MB hard disk, IBM parallel/serial card, standard "AT" keyboard (IBM system 5170-099) an EGA Graphics Card (IBM option 1200), an EGA Color Monitor (IBM 5154-001), and IBM DOS 3.1 PC System Software.

An Epson LX-86 printer, normally used with the SpectrAA, was connected to the IBM PC parallel printer port using an IBM centronics cable (01-103498-00) for printouts from Lotus.

Two readily available IBM PC programs were used to store and manipulate the SpectrAA data on the IBM system:

1. Kermit (version MS V2.27) – a public domain communications program
2. Lotus 1-2-3 (version 2.0), a widely used commercial spreadsheet package

For fully automatic data transfer, a duplicate of the SpectrAA 40P flame system disk was configured as described below. This allowed the operator to choose between normal operation (hard copy on the SpectrAA printer using the standard system disk) or data output via RS-232C using the configured system disk.

## System Disk Configuration for Data Transfer

The SpectrAA flame and furnace system disks may be configured to transfer data automatically to external computers. This is achieved with the Agilent Technologies communications software (supplied with the communications interface) as shown in Figure 1.

Thus, once a system disk is configured as a communications disk (a once-only operation), a routine analysis can be carried out on the SpectrAA 40P (and similarly for other SpectrAA models) simply by selecting either "develop method" or "automatic run" on the program modes screen as shown in Figure 2. Alternatively, the analytical data can be archived using the optional SpectrAA Utilities program and sent to the IBM PC at any later date using the SpectrAA "Print Reports" facility.

## Multi-Element Analysis Set-Up SpectrAA-40 P

The analysis of 16 composite daily samples for their concentrations of copper, iron and lead was set up for flame atomic absorption analysis on a SpectrAA 40P instrument, equipped with a PSC-56 automatic sample changer, in a fully automatic sequence.

Prior to starting the analysis, the SpectrAA report format was set for a multi-element report using the parameters shown in Figure 2.

## Data Transfer of a Multi-Element Analysis from SpectrAA to the IBM PC/AT

The Kermit communications program was then set up at the IBM to receive and store the resulting SpectrAA data. These steps instructed the IBM to:

1. Configure the Kermit program to receive data via RS-232 using the correct protocol
2. Assign a text file (called RESULTS.PRN) for data storage
3. Await on-line data transfer

Commands entered at IBM	Remarks
KERMIT	loads the Kermit program
SET PORT 1	sets the IBM to receive on Comms Port 1
SET BAUD 2400	sets correct baud rate via RS-232C
SET PARITY N	sets RS-232C parity condition
LOG RESULTS PRN	assigns a file to storage of results
CONNECT	ready to receive RS-232 data

At this stage, the Kermit program will wait to receive data from the SpectrAA. The analysis was then initiated at the SpectrAA, and at the end of the run the SpectrAA multi-element report was automatically transferred to the IBM, listed on the IBM screen and stored by the Kermit program (shown in Figure 3). Upon completion, the Kermit program was logged off-line using the following instructions at the IBM keyboard:

Ctrl-] C	Hold Ctrl key down, press ] key, then lift both keys and press C key
EXIT	closes file and exits from the Kermit program

## Lotus Spreadsheet Manipulations

The SpectrAA multi-element report (stored by Kermit under the filename RESULTS.PRN) was loaded into the Lotus 1-2-3 spreadsheet and manipulated to provide a simple trend of day-to-day metal concentration.

The following brief description of data manipulation is provided for users familiar with Lotus 1-2-3 software, version 2.

Prior to loading the SpectrAA report, the Lotus worksheet cell position was set to an unused portion of the spreadsheet, for example, cell Q1 and the Lotus "File Import Text" commands were used to load the SpectrAA Report.

To format the report for numerical calculations, the Lotus "Data Parse" commands were used to reformat the sample results column into separate cell fields for sample number, and individual multi-element concentrations. The parsed data and report header were then copied to the start of the worksheet (shown in Figure 4).

To plot a trend graph, where each sample represented a daily analysis, a line graph was chosen using the sample number as the X axis, and the Pb, Cu and Fe columns as the A, B and C axis, respectively.

After adding suitable axis legends and titles, the graph in Figure 5 was produced. An alternative graph display was also produced using the Lotus stacked bar graph type to display total metal content in the day to day samples (shown in Figure 6). Other graph formats can also be readily produced according to the operators requirements.

## **Conclusion**

The transfer of analytical data from modern spectrometers such as the Varian SpectrAA Series, to external computers can be easily performed using the Varian communications facilities in conjunction with readily available IBM communications software such as Kermit.

The availability of powerful PC software such as Lotus 1-2-3 enables laboratories to process spectrometer data off-line for additional report capabilities and statistical analysis. Furthermore, the MACRO capability of Lotus allows the analyst to pre-program the calculations to be performed automatically within Lotus, avoiding the need for detailed knowledge of Lotus operation by day to day operators.

The examples given in this At Work clearly illustrate the usefulness of commercially available spreadsheet software for the manipulation and generation of analytical reports tailored to individual laboratory needs.

## **Acknowledgement**

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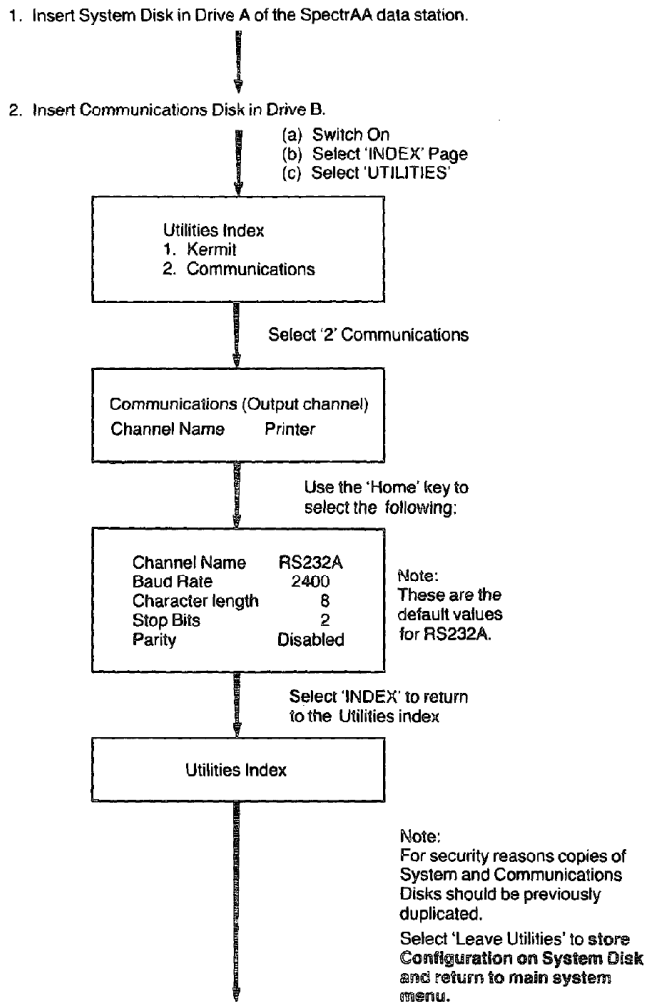


Figure 1. Configuring the SpectrAA 40 for RS-232 data transfer.

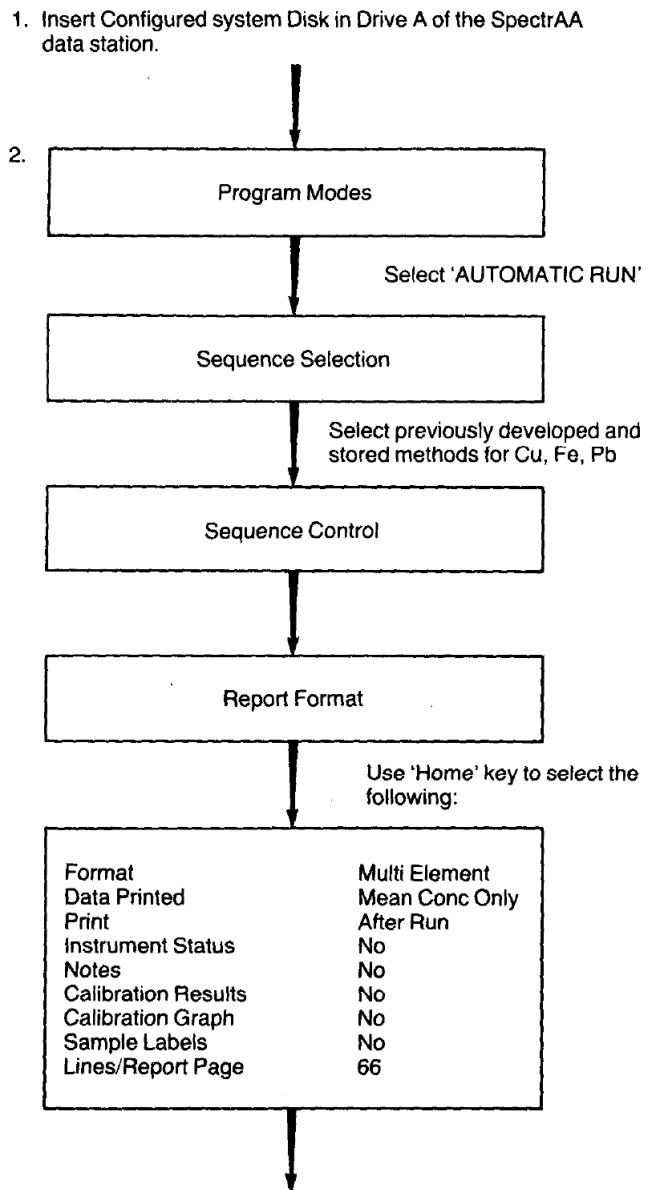


Figure 2. Steps for day to day analysis and automatic data transfer to IBM.

```

OPERATOR      JD/SS
DATE          21 Oct
BATCH         Cu/Pb/Fe Analysis

PROGRAM 11   Pb  LOCO OIL
PROGRAM 1    Cu  LOCO OIL
PROGRAM 12   Fe  LOCO OIL

```

		Pb ppm	Cu ppm	Fe ppm
SAMPLE	1	10.22	2.25	4.64
SAMPLE	2	12.68	2.82	7.65
SAMPLE	3	10.70	2.09	5.78
SAMPLE	4	8.67	2.18	4.23
SAMPLE	5	12.88	2.43	5.92
SAMPLE	6	13.83	0.88	5.56
SAMPLE	7	10.33	2.96	6.78
SAMPLE	8	9.96	2.65	6.23
SAMPLE	9	10.55	2.12	9.92
SAMPLE	10	11.68	1.44	7.23
SAMPLE	11	10.23	3.45	5.97
SAMPLE	12	8.24	3.45	7.88
SAMPLE	13	9.96	4.52	6.44
SAMPLE	14	11.87	1.33	7.87
SAMPLE	15	18.85	2.35	6.63
SAMPLE	16	16.21	4.03	8.54

Figure 3. SpectrAA report, transferred and stored on IBM PC under Kermit.

```

A10: [W9]          BATCH          Cu/Pb/Fe Analysis          MENU
Worksheet Range Copy Move File Print Graph Data System Quit
Global, Insert, Delete, Column, Erase, Titles, Window, Status, Page
  A      B      C      D      E      F      G      H
8      OPERATOR      JD/SS
9      DATE          21 Oct
10     BATCH         Cu/Pb/Fe Analysis
11
12     PROGRAM 11   Pb  LOCO OIL
13     PROGRAM 1    Cu  LOCO OIL
14     PROGRAM 12   Fe  LOCO OIL
15
16           Pb      Cu      Fe
17           ppm     ppm     ppm
18
19 SAMPLE      1    10.22    2.25    4.64
20 SAMPLE      2    12.68    2.82    7.65
21 SAMPLE      3    10.70    2.09    5.78
22 SAMPLE      4     8.67    2.18    4.23
23 SAMPLE      5    12.88    2.43    5.92
24 SAMPLE      6    13.83    0.88    5.56
25 SAMPLE      7    10.33    2.96    6.78
26 SAMPLE      8     9.96    2.65    6.23
27 SAMPLE      9    10.55    2.12    9.92
21-Oct-86  01:05 PM

```

Figure 4. SpectrAA results, viewed in Lotus 1-2-3, after formatting.

### Monthly Trend Analysis

Daily Pb/Cu/Fe Concentrations

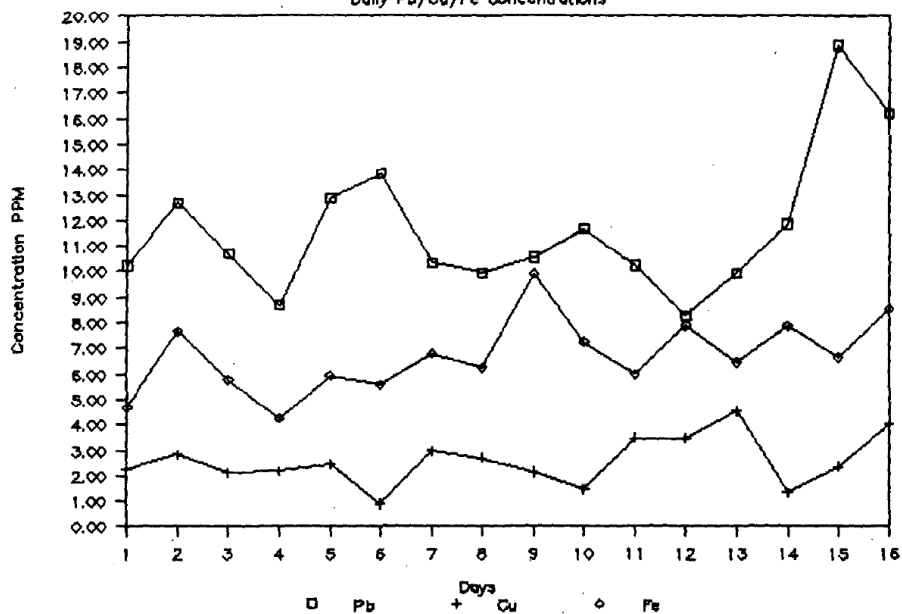


Figure 5. Trend graph from Lotus 1-2-3, using tine graph.

### Monthly Trend Analysis

Daily Pb/Cu/Fe Concentrations

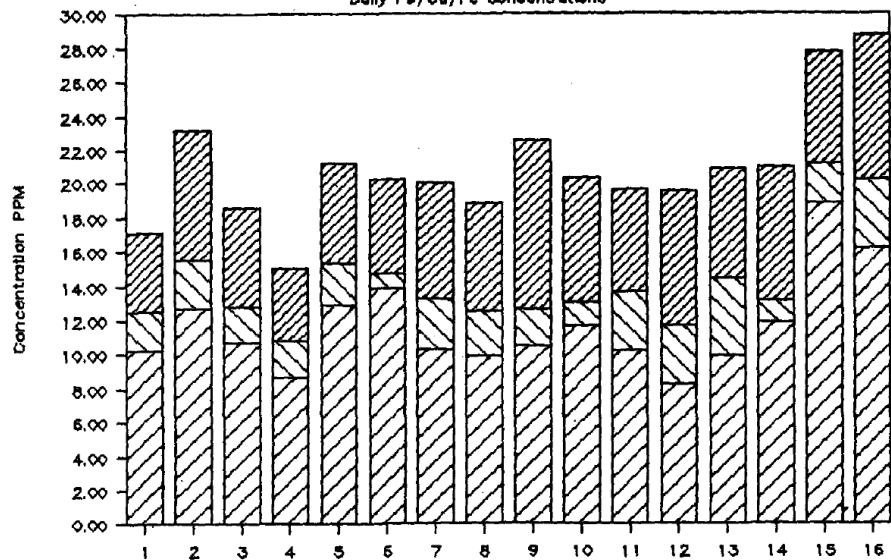


Figure 6. Trend graph from Lotus 1-2-3, using stacked bar graph.

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