Chapter 2

Data Acquisition and Device Control

2.1 INTRODUCTION

Numerous papers have been devoted to the use of microprocessor-controlled flow-injection analysis (FIA)[1]. Different aspects of the control of FIA systems have been described. Most authors agree that computer control and data acquisition leads to superior results and improved use of this versatile method of sample manipulation. In the author's laboratories, there was a need for a software package that would satisfy the requirements of several different groups of people, *viz.* research scientists, service analysts, and plant analysts. The possibility of using one package both in the laboratory environment for research, method development, and service analysis, and in the plant environment for process analysis has not been adequately addressed in commercially available packages. Such an approach demands a modular design and adaptable user-defined set-up options. Integration of the hardware and software must be such as to afford maximum flexibility and user-selectable configuration. This level of flexibility is often absent in commercial systems where the requirement for simplicity places constraints on flexibility.

The researcher demands a system by which simple and flexible configuration of the manifold, single measurements under various conditions and comparison of the resultant peak profiles, the use of a variety of devices and detectors, repeated performance testing, and convenient system documentation are all easily achieved. The service analyst, on the other hand, needs a reliable data acquisition system with the facility to load and save standard methods of analysis. The ability to control an auto sampler is also important. The process analyst, in turn, requires a system that can repeat a measurement at a predetermined frequency, with the added feature of being able to specify a sequence of measurement methods or sub procedures, e.g., calibration, followed by several measurements, and then a wash sequence. (This approach to process analysis will be discussed in more detail below.) The facility of allowing certain basic instrumental diagnostic tests should not be excluded for the process analyzer.

One of the attributes of FIA is that it is reasonably simple and inexpensive to purchase or to build components and assemble these into an FIA manifold This has lead to the wide use of in-house systems. These systems can be operated manually with detector output being directed to a chart recorder. This approach is even used in primitive service laboratories. However, the additional advantages of manpower saving and improved quality of data can be achieved through the coupling of the FIA system to a computer for automated device control and data acquisition.

In the study of sequential-injection analysis (SIA)[2] it quickly became apparent that micro-processor control was mandatory. In this novel technique by which the familiar manual laboratory processes of mixing various reagents and carrying them to a suitable detector is automated in a flow system, precise control of a sequence of events ensures reproducible and accurate results. Although this technique can be implemented in the laboratory, its primary application will likely be in the plant environment. In this environment, the ability to manipulate the data and turn it into useful process monitoring or control data should also be incorporated in the device control and data acquisition package. Also, the use of SIA in sensor-based systems will greatly enhance the usefulness of these sensors. Research into the technique and its various applications as well as method development will still take place in the analytical laboratory. Our requirement for a versatile package was therefore extended to include computer control and data acquisition for the related technique of SIA both for the process environment and in the research laboratory. The need for a package that would satisfy all of these requirements prompted the development of this software package.

2.2 INSTRUMENTAL DESIGN

A definition of the terminology used in this chapter and the program is given in the glossary at the end of the chapter.

2.2.1 *Computer*

This program was written for an IBM PC (or compatible) with an enhanced graphics adaptor (EGA) or visual graphics array (VGA) screen. A minimum of 256 kilobytes random access memory (RAM) is required. Although the program can be run on a computer equipped with a 360 kilobyte floppy disk, this places a limit on the number of data files that can be saved and has certain speed implications. The program has been written for the DOS environment but will run in a DOS shell of the Windows environment.

2.2.2 *Interface board*

A general-purpose analog and digital input/output interface board (PC-30B from Eagle Electric, Cape Town, South Africa) was used to interface the computer to the analytical instrumentation. Subsequently the facility to interface other boards, notably the ADA 2200 (Real Time Devices), was also added. Support for other interface boards is simplified by the modularity of the program structure which ensures that all interface-specific commands are kept together. The minimum specifications of this board are set out in Table I.

In the planning of this program's architecture, particular attention was given to maintaining modularity and including user-definable flexibility. These two requirements were not allowed to compromise requirements for a simple and user-friendly interface.

Facilities are provided for the connection of up to eight user-definable devices (e.g., pumps, valves, on/off switches) to digital output points. Four digital input points are configured to enable a measure of instrument diagnostics (e.g., to test whether the reagent reservoir is empty) or other diagnostic signals to the software. Four analog input ports allow for a maximum of four detector or other analog devices to be sampled by the program. Figure 5a illustrates the relationship between the computer and analytical apparatus for FIA. The relationship between the computer and analytical apparatus for SIA is given in Figure 5b.

Table I

Minimum specifications for FlowTEK *interface board*

(satisfied by the PC-30B and ADA 2200 interface boards)

Analog input channels	4 single ended (12 unused by the program)
	12-bit resolution
	Input range (0 to 10 V)
	Input impedance (>100 kΩ/100 p)
	Acquisition rate ($3x10^4$ sec^{-1} variable)
Digital I/O	24 in 3 ports programmable as Input or Output
	TTL compatible
Required power	100 mA at ± 5V
PC connection	Uses a fully bussed full length 8-bit slot of an
	80x86 computer

2.2.3 *Distribution board*

A distribution board was built which allows for easy connection of the devices and detectors to the interface board. A variable gain amplifier circuit was included on this distribution board to enable connection to analog devices with an output range and offset different to that available on the interface board. (This variable gain amplifier allows signals as low as 0 to 10 mV to be amplified 1000 times and an offset of ±12 V

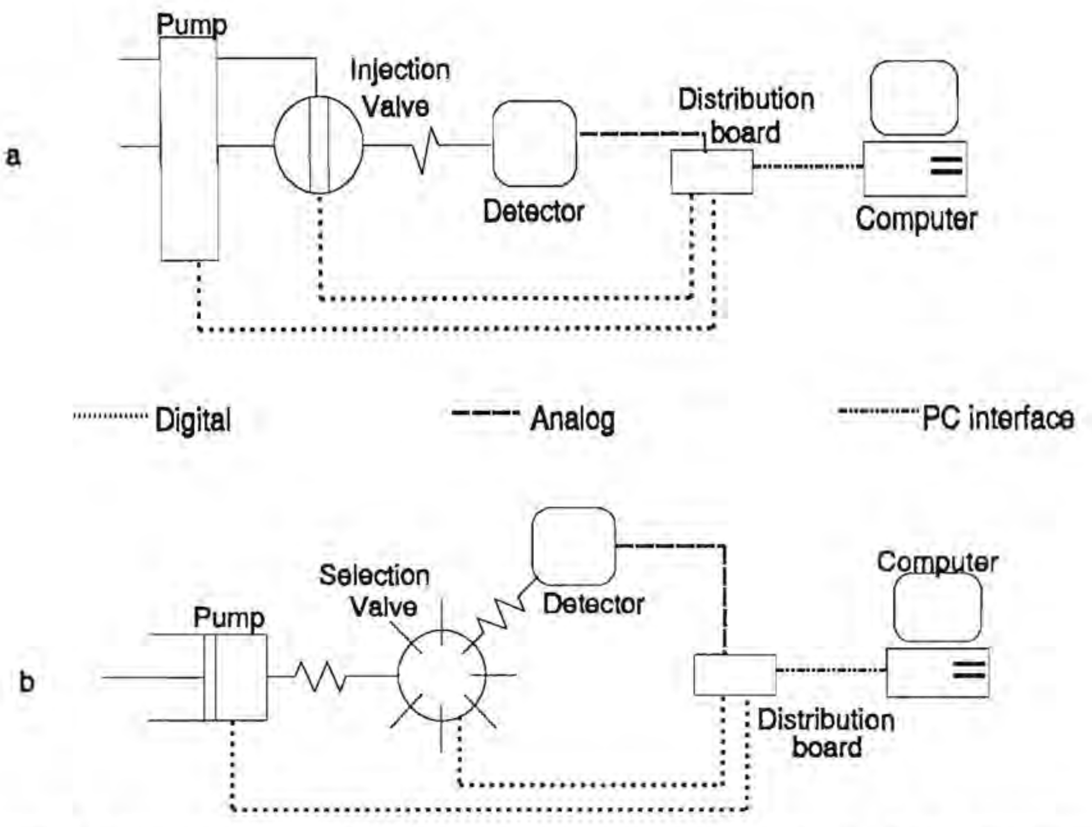

Figure 5: Manifolds and their relationship to computer hardware. a. Flow-injection manifold. b. Sequential-injection manifold.

to be eliminated.) Incorporated in the amplifier circuitry are three levels of electronic filtering with time constants of 0.01, 0.1, and 1 second. Equipped with this electronic signal smoothing facility, it was not necessary to include any signal smoothing routines in the software. These of course can be applied to the raw data using a third party package.

Circuitry was added to the digital I/O lines to enable both TTL and switch control of digital input and output signals.

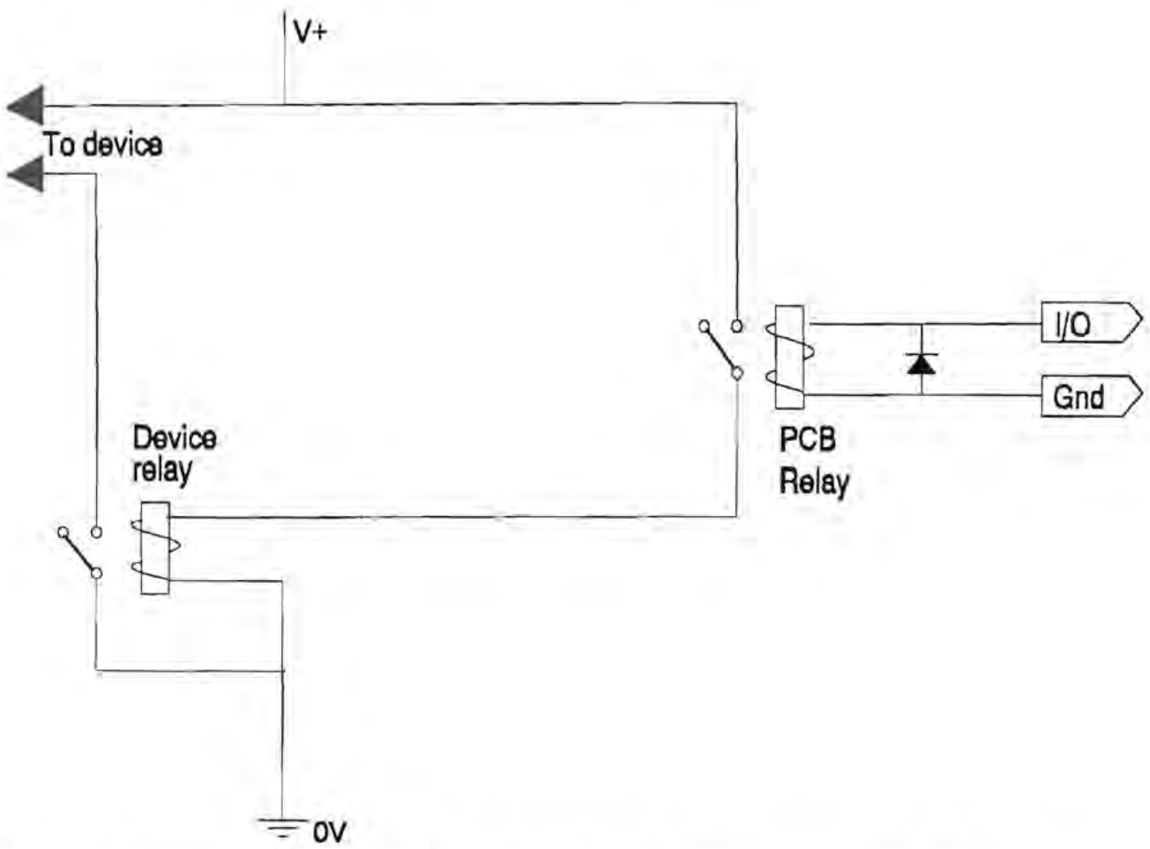

Figure 6: External relay for devices without built-in TTL control. The PCB relay is equipped with a coil of 5V and 500 Ω.

Some of the features described by Clark *et al*[3] in a similar program were implemented in this program. The main differences in the user interface between this package and that of Clark *et al* are in the Methods development module. Features which greatly simplify the definition of methods, particularly for SIA, have been included. Of particular note is the ability to "insert time" between events. This facility is required because in SIA experiments, volume of reagents and sample aspirated is determined by time[2,4]. The data handling facilities of this package have also been enhanced, and more user-defined options are provided.

The modularity of the program was achieved by the independent development and debugging of 20 source files. The source files were compiled and linked using the

Turbo C++ Project Make facility (Borland Corp. Scotts Valley, CA, USA). Figure 8 gives the dendrogram of the program. Each level in the program is activated through menu choices. Menu options are chosen by hitting the key corresponding to the first letter of the menu choice. The main menu is shown in Table II. Each option can have sub-menus below it. Progress back towards the main menu is achieved by hitting Esc or Q for Quit.

The configuration selected by the user is saved to a configuration file on exiting the program. This configuration file is read at the start-up of the program, thereby ensuring the maintenance of the experimental environment from one session to the next. Of course, changes to the configuration are easily achieved through the various menu options. The current state of all user-selected parameters may be displayed on the screen, or as a hard copy on the printer, with the Note Pad menu choice. The parameters that are saved in the configuration file are listed in Table III. At start-up, the last used method file and calibration set up parameters are also read thus ensuring continuity from one experimental session to the next..

Table II

Main Menu Options

Menu option	Description
Once	Executes a single measurement
Repeated	Executes a procedure resulting in several measurements
Calibrate	Performs a least squares regression using either an exponential, rectangular hyperbola, or first, second, or third order model on one of the peak parameters (peak height, area, time, or width at a specific height)
History	Displays one of the peak parameters for up to one hundred measurements
Method	Defines an experiment method allowing various device events to be programmed, e.g., pump off after x seconds, inject at y seconds, detector off, etc.
File	Allows various file name selections and manipulations such as delete, directory and a shell to the disk operating system
Setup	Provides for basic user choices such as mode of auto zero operation, integration limits, the number of detector, and screen display options
Notepad	Lists the present settings for all user-selected options
Quit	Exit from the program

Table III

User-selected configuration parameters and program defaults

Parameter	Default
Path	c:\flowtek\data
Reduced data file	default.red
Method file	default.met
Calibration file	default.cal
Profile file root	default
Save all profiles	Yes
Main procedure file	None
Detector display mode	Paged
Re-scale y axis	Yes
Initial y axis range (arbitrary units)	-0.005 to 1.0
Number of detectors	1
For each detector:	
Minimum integration limit (sec)	0
Maximum integration limit (sec)	60
Height at which width is measured (arbitrary units)	0.1
Time at which peak height is measured (sec)	At peak maximum
Auto zero mode	Every measurement
Time at which zero response is measured (sec)	0
Auto zero offset	0

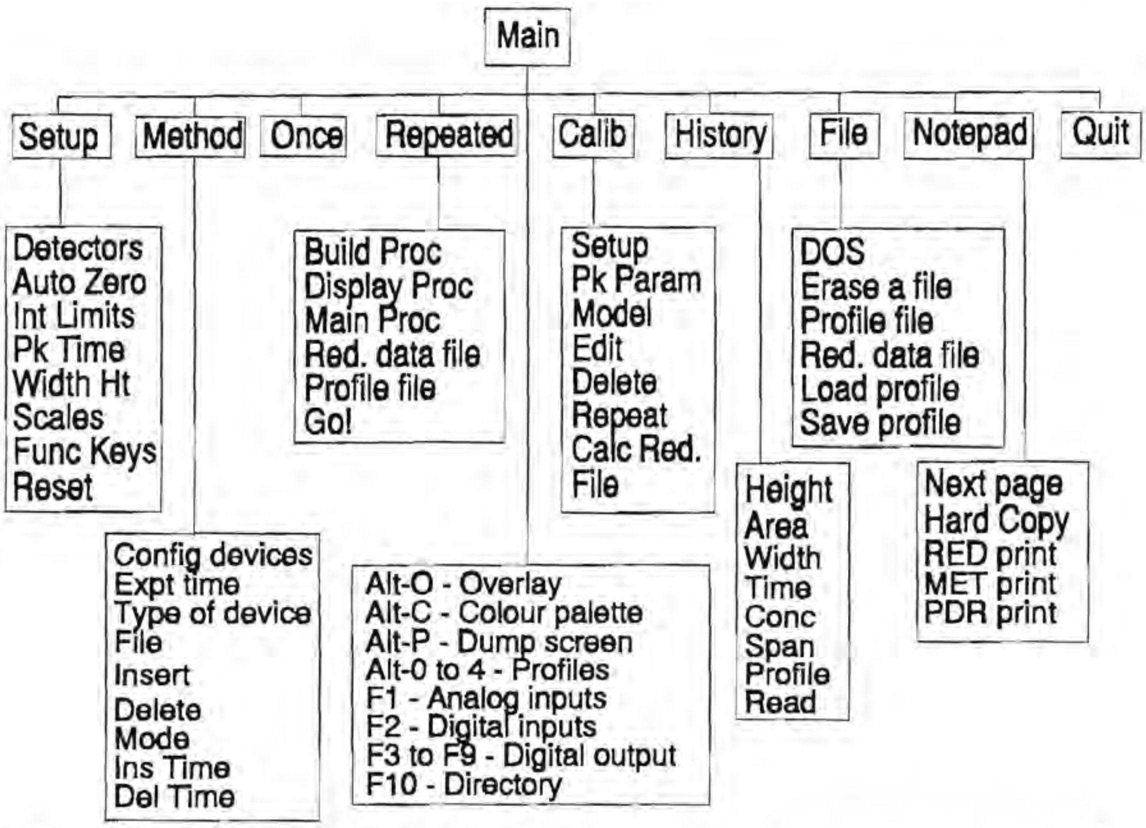

Figure 7: Dendrogram of FlowTEK program showing the various menu options and program functions.

Figure 8 represents an image of the main screen. The top line is reserved for the menu options. The second line is for user input when prompted, and messages from the program. The rest of the screen is divided into four boxes, three of which are always visible. As data are collected, they are plotted in real time as a peak profile in the profile box. The present value of the response and time is also given in a box which appears during each measurement. The scale on the time and response axes can be selected to best display the peak profile. On completion of the measurement, the peak parameter box is updated. This peak parameter box provides useful information which is not easily obtained from a chart recorder plot, *viz.* peak height ,peak area, peak width at a particular height, peak time, and concentration. A line diagram in the device box depicts the state of each of the manifold devices during the experiment.

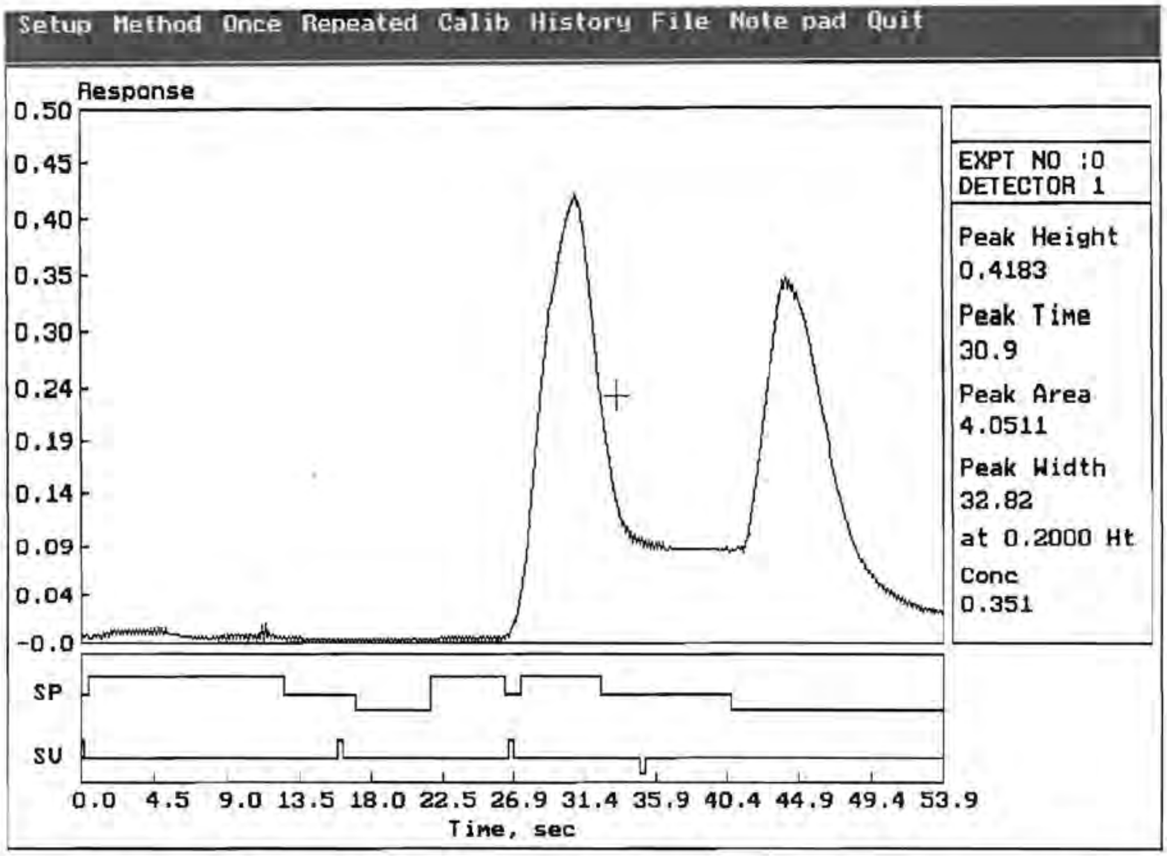

Figure 8: Typical flow-injection profile as depicted on the Main menu screen. Note the device events are depicted schematically in the device display box.

The scaled time and response co-ordinates of a cross-hair cursor are given in the fourth box, which becomes visible if the arrow-key-driven cross-hair cursor is activated between measurements. This facility is useful to pinpoint the actual response at a given time, or the exact time of a particular response phenomenon.

A peak overlay facility is activated with a hot key. This facility enables subsequent profiles to be overlaid in different colours instead of clearing the screen between each measurement. This option has proved most useful in the research environment where peak shape provides additional diagnostic information. In fact, it is our experience that the amount of diagnostic information provided by this approach is far superior to that obtained from a chart recorder.

The peak parameters (height, area, width, time, and concentration) together with the date and time of the measurement, the profile file name, and method name are stored in one data file called the 'Reduced Data' file (see Table IV for an example). The entire profile, together with the program parameters used in the experiment, as well as just the profile data can be stored for each measurement. The file containing just the profile data is called the abridged profile file and is useful when importing profile data into third party packages for further data manipulation of the response data. These data are stored as the original analog-to-digital raw data. Numbers are therefore integers in the range 0 to 4095. Experiment profiles may be recalled and displayed for comparison in up to four pop-up windows on the main screen. Alternatively they may be overlaid in the main response profile box.

Methods are stored in method files. The definition and design of methods are discussed in more detail below. Procedures are stored in procedure files. (A procedure is a list containing other procedures, methods and wait periods.) Procedures provide a powerful facility for the control of experiments. The use of Procedures is described in more detail below.

Table IV

Typical FlowTEK *Reduced data file*

Date	Time	Peak Height	Peak Time	Peak Area	Peak Width	Width Height	Conc	Profile File	Method File
1994-04-14	16:48:12	2.5513	36.26	17.0731	5.69	1.00	0.0000	DEFAULT1.1	SIACN1.MET
1994-04-14	16:49:10	2.5073	36.15	21.0239	5.81	1.00	0.0000	DEFAULT1.2	SIACN1.MET
1994-04-14	16:50:08	2.4658	35.93	22.5973	5.71	1.00	0.0000	DEFAULT1.3	SIACN1.MET
1994-04-14	16:51:06	2.8906	35.60	24.7214	6.37	1.00	0.0000	DEFAULT1.4	SIACN2.MET
1994-04-14	16:52:03	2.7856	35.93	24.2471	6.22	1.00	0.0000	DEFAULT1.5	SIACN2.MET
1994-04-14	16:53:01	2.7173	36.48	22.9830	6.40	1.00	0.0000	DEFAULT1.6	SIACN2.MET
1994-04-14	16:53:59	2.9272	35.82	27.2263	7.74	1.00	0.0000	DEFAULT1.7	SIACN3.MET
1994-04-14	16:54:57	2.9053	35.82	25.7511	7.04	1.00	0.0000	DEFAULT1.8	SIACN3.MET
1994-04-14	16:55:53	2.8223	36.81	25.2674	7.42	1.00	0.0000	DEFAULT1.9	SIACN3.MET

All data files are stored in American standard code for information interchange (ASCII) format. This feature is particularly important for the reduced data file and peak profile file, since it facilitates the importing of the data from these files into any editor, statistical package, or spreadsheet package. A macro-driven spreadsheet for Quattro Pro has been written that imports the data from the reduced data file and places each number or label in its respective cell in the spreadsheet. Graphing and statistical macros are envisaged for this spreadsheet. This mode of operation can also be used to produce user-defined reports.

2.4 METHOD DESIGN AND DEVELOPMENT

A method in this program consists of a list of device events and the time (in seconds), after the start of an experiment, that the event should occur. In addition, information such as the duration of the measurement, time after the start of an experiment that data collection should begin, and various set-up options such as the integration limits and auto-zero mode also form part of the method. Up to eight devices may be defined in each method. Each device can assume one of up to three digital states (e.g., for a pump the three states of forward, off, and reverse can be defined). Analog control of devices (e.g., programable control of pump speed) has not been included. For devices which require more than three states, a single device can be spread over more digital output points.

When the method option is chosen from the main menu, a new screen is obtained which provides a full screen representation of the line diagram in the device box on the main screen. In addition, another box is provided which lists the actual event time and actions for each device. On this page, the devices used are defined and the duration of the measurement is selected. A cross-hair cursor is used to insert and delete events. Alternatively, the absolute time and device choice may be entered from the keyboard. For example, in response to prompts, the user would respond with the characters in bold print, at time **0** set device **1**, the pump, **F**orward and device **2**, the injection valve, to the **L**oad position. The "Insert" and "Delete" keys are used to insert or delete time between events. This option is useful during method development in the optimization of the method. It also proved to be essential in SIA where time determines volumes of selected reagents and samples. Method files can be saved and retrieved for later use or inclusion in a procedure.

2.5 Data Acquisition and Instrument Control

On execution of a measurement, a loop is entered in the program that consists of three tests. This loop is executed at maximum speed until the time set for the measurement has passed.

The first test establishes whether a device event should occur. If so, the necessary value is sent to the relevant digital output port to execute the event. The status of the port before an event is maintained by the software to ensure that an event on one device does not change the present status of the other devices linked to that port. The required output values and the time at which they are to occur are calculated and stored in an array when the method file is loaded.

The second test in the data acquisition and device control loop monitors the keyboard to establish whether the "Esc" key has been pressed. The "Esc" key aborts the measurement and returns control to the main menu. All other input from the keyboard is ignored.

The third test determines whether 0.1 second has elapsed since the last collected data point. If so, the next data point is collected for each detector. If not, the data collection routine is skipped. Each data point is not simply a single reading from the analog-to-digital (A/D) converter. The PC-30B interface board is equipped with a 12-bit monolithic A/D converter. The board contains logic which allows any sequence of the 16 channels to be sampled. (A maximum of four channels are allowed in this program.) Use is made of the direct memory access (DMA) mode of data collection. In this mode, the selected channels (usually only one) are sampled at the maximum data acquisition rate (3×10^4 sec^{-1}) until sixteen values have been obtained for each selected channel. These digital values are stored directly in the computers memory at an address passed to the data acquisition sub-routine. The maximum elapsed time in the collection of this data when four channels are used is 2.13×10^{-3} sec. For practical purposes, this data is collected instantaneously. On completion of the direct memory storage of the acquired data, the data for each channel are sorted and the two highest and two lowest values are discarded. It is assumed that these may be outliers. The response for each channel is then calculated as the average of the remaining values.

In this way, a data point for each of the detectors is obtained every 0.1 second. However, that data point represents the average of the 12 middle values from 16 values acquired at the maximum acquisition rate. A user-selected mathematical function is then applied to the response from the detector (e.g., transmission data can be converted to absorbance) and the resultant point is plotted on the screen. The Response-Time box is also updated every 0.5 seconds.

At the end of measurement, a calculation routine is executed. In this routine, the user's choice for auto-zero is implemented. By auto-zero, we mean that a zero offset is subtracted from every data point. The value subtracted is obtained at a user-specified time during the measurement (usually at the start of the experiment). The user also chooses whether this auto-zero option is to be implemented and if so, whether a new offset is obtained for every measurement or just at the start of the procedure. Having implemented the desired auto-zero calculation, the peak height, time of peak maximum, peak area, peak width at a specified height, and concentration are calculated.

For peak height measurement, two options exist. Either the maximum height of the peak is given, or the height at a specified time after the start of the measurement is determined. This enables the implementation of the so-called electronic dilution method[5]. The peak time is then set at either the time at which the peak maximum occurred or the chosen time after the experiment starts. Peak area is determined by Simpson's rule (reviewed in ref. 6). Peak width at a specified height is a useful parameter in FIA titration[1]. If certain manifold design rules have been observed[1], concentration of the sample (C_s) is related to peak width (Δt) according to the following proportionality:

$$\Delta t \propto \log_{10} C_s$$

If a calibration calculation has been performed or a calibration file has been loaded, the concentration of the analyte in the sample can be determined using the calculated regression coefficients and the chosen peak parameter. If no calibration has been carried out, the regression coefficients are taken to be zero, i.e. a concentration of zero is reported.

2.6 CONTROL BY PROCEDURES

In the Repeated mode of operation, a Main Procedure file is defined and executed. The main procedure consists of a combination of other procedures, methods, and a WAIT operation which allows a pause (of up to 8 hours) between measurements or until a digital input is received at a particular digital input point. This option is of particular use in the process environment where the maximum analysis throughput may not be required or an external event may signal the need for a measurement. On initiating a procedure, an algorithm that makes use of a stack structure is executed until the end of the main procedure is encountered. This structure allows nested procedures. (Recursive calls of a single procedure will however result in a stack overflow.)

The facility of being able to define and execute a procedure is an extremely useful one. It allows the analyst to define the sequence of events in an analysis scheme. This means that it is no longer necessary for the same method to be executed repeatedly. However, by design of a suitable procedure, various useful options may be included. For example, standards may be analyzed in duplicate in a calibration procedure. This could be followed by a measurement procedure which analyses each sample in triplicate (samples could, of course, be drawn from one of several sources), and after every 10 samples, a wash method could be executed. The main procedure could be concluded with a repeat of the calibration procedure (to test calibration validity) and a short method at the end to flush the tubing with wash solution and switch off the various devices. The procedure can be aborted at any time by using the "Esc" key. Countless variations on this theme can be developed. The use of procedures opens the option of leaving the analyzer unattended in the process environment or, together with an autosampler, for overnight laboratory use. It also provides the researcher with the ability to acquire data without necessarily being in attendance. This means that the researcher can busy himself in a more productive fashion.

The reduced data file, containing the peak parameter values for each measurement in the procedure, also contains the method file name used to generate the data. This, together with the time of analysis, allows for adequate sample identification. The reduced data file also keeps a record of the profile file name. The full peak profile for each measurement can be saved. This allows the user to investigate unexpected results at the end of a procedure by looking at the peak profiles.

2.7 CALIBRATION

Several user-selected options have been included in the calibration routine.

- The data used for the calibration can be selected from any reduced data file. The only prerequisite is that the data form a contiguous block in the reduced data file. Alternatively, the user may type in calibration data from the keyboard.
- Up to five standards may be used.
- Each standard can be analyzed once, in duplicate, or in triplicate. Where more than one reading is taken for a particular concentration, the spread of readings

are depicted on the calibration graph. The regression calculation uses the arithmetic mean of the readings.

- The regression can be carried out on any of the peak parameters.
- A least-squares regression using either a linear, quadratic, cubic, exponential, or rectangular hyperbola model is performed on the calibration data. Another option allows for all five models to be applied. The model which gives the best correlation coefficient (r^2) is then adopted.

The regression coefficients and calculated correlation coefficient are displayed together with all the calibration data. The calibration curve is also displayed for visual inspection and evaluation of the regression model applied to the data.

Two methods of editing the data, besides the manual entry of data from the keyboard, are presented. In the first case, a simple deletion of any data point is allowed (provided that there are sufficient data for the selected model). Deleted points are marked as deleted for future reference. In the second case, any measurement may be repeated, and the new data value replaces the old.

2.8 Diagnostics using the History option

A facility is provided to display graphically, as points or bars, any one of the peak parameters. A maximum of 100 measurements from a reduced data file can be displayed. A cross-hair cursor allows for any measurement to be selected and all the peak parameters for that measurement to be displayed in a peak parameter box. The profile, if it were saved for the experiment, may also be conveniently recalled and viewed in a pop-up window.

This menu option provides a pseudo chart recorder type of display, but has the added advantage of allowing any of the peak parameters to be displayed. The display of the profile allows a closer *post mortem* examination of the profile of a measurement of particular interest.

2.9 SYSTEM PERFORMANCE

The program has been tested in both flow-injection and sequential-injection applications where it was used for automated data acquisition and device control. The repeatable control of the devices improved the precision and accuracy of the data. In one application, the program was used to synchronize pump events in a dilution method described by Clark *et al*[7]. The precision attained improved by about an order of magnitude when electronic control was used.

2.9.1 *Study of fundamental parameters*

The software went beyond enabling researchers to duplicate, in a more convenient fashion, what they were already doing manually.

- Of course, the tedium of a simple manual task such as injecting a sample slug into a flowing stream was removed from the user and left to the computer.
- More importantly though, the software opened up areas of endeavour and research not previously possible. For example, the technique of flow reversal, where the sample is oscillated back and forth in the reaction tube before being dispelled to the detector, can only be investigated with the aid of computer control.
- Of greater consequence for the present investigation, precise computer control is the foundation on which SIA is built. Volumes are determined by accurate control of pumping times. Complex selection valve programmes are routinely and repeatably handled by the software without any intervention by the researcher.
- Having the flow-injection or sequential-injection profile stored on electronic media makes the manipulation of the data using third party packages both feasible and most enlightening.
- Research and method development requires making continual changes to the method employed. The convenient graphical user interface proves invaluable in this regard. In particular for SIA, the facility of being able to insert and delete time between device events and thereby change the respective volumes, was found to be particularly useful. Investigations into the effect of sample volume, for example, are directly affected by this option.

2.9.2 *Method development*

The investigation of the suitability of various chemistries for the analysis of a particular sample or the development of a new method of analysis from sound principles of chemistry, is conveniently handled by the package whether the chosen platform is flow-injection or sequential-injection analysis.

- Methods (as used in FlowTEK - see the glossary for the definition) are conveniently constructed and optimized using the Method menu option.
- Interference studies are simplified with the flexible profile recall facilities and trend monitoring using the History menu option.
- Various calibration models can be investigated and compared.
- Analytical figures of merit such as precision, working range, sample throughput, and detection limits are derived from data stored on electronic media in the reduced data file.
- Once established, a hard copy of Methods, and other key configuration parameters can be produced for inclusion in the investigators note book.

2.9.3 *Flow-based analysis as a diagnostic research tool*

Some workers have used flow-based analysis to track the progress of a particular experiment. A good example of this was the investigation of various aspects of supported liquid membranes (SLMs) using flow-based analysis. Barnes[8] made extensive use of this software to optimize the composition of the membrane, study the formation and degradation of an SLM, and explore transport mechanisms, as well as parameters such a membrane geometry. Again the availability of key data in electronic format and the ability to leave the experiment unattended to gather data over extended periods proved most valuable.

2.9.4 *Service analysis*

While the software conveniently handles the acquisition of data in a service laboratory environment, manipulation of the data and report writing is best handled by a third party package such as a spread sheet package. Nevertheless, the repeatability of computer control improves the quality of analytical results by removing the influence of poor duplication. Also analyst errors are effectively eliminated.

2.10 FUTURE DEVELOPMENTS

2.10.1 Windows™ *platform*

With proliferation of the Windows operating environment, it is inevitable that users of the software will require the porting of the software to the Windows platform. In such an upgrade, specific attention will be given to exploiting the power of the graphical user interface to simplify the configuration, utilization, and understanding of flow-based analysis. Data manipulation and report writing tools, already available in the Windows environment, must be tapped to enhance the power of the package in these areas.

Options should be developed with both the researcher, routine laboratory analyst, and process analyst in mind.

2.10.2 *Sequential-injection analysis*

Research in SIA in the future is likely to centre around three areas:

1) Application development.
2) Operational simplification and manifold miniaturization.
3) The development of sample manipulation capabilities for sensors.

Software which streamlines research in these areas will contribute significantly to the development and general acceptance of SIA. As pumps are developed and improved, a comparison of time-control of SIA experiments with volume-control will necessitate the addition of a module to the method routine. This routine should also allow the random selection of selection valve ports. (At present valve ports are accessed sequentially.)

2.10.3 *System configuration*

Flow-based analysis techniques frequently require the user to configure the manifold for a particular measurement. Some instrument suppliers have dealt with this by providing encoded manifold cartridges which are simply slotted into a chassis and automatically configure the software for the required measurement. While this level of automated system configuration is appropriate in many environments, it does remove a level of flexibility (which has always been regarded as a positive characteristic of flow-based analysis) from the analyst. A software package which allows intuitive configuration of the manifold and even provides expert comments on manifold design would provide the best of both worlds.

2.10.4 *Multi-array detectors*

A major field of endeavour in research into flow-based techniques in the coming years will be centred on the use of multi-array detectors such as diode array spectrophotometers and arrays of sparingly selective electrodes. Future software will have to allow the acquisition and manipulation of multi-channel detector output.

2.10.5 *Process monitoring and control*

The incorporation of a third construct in Procedures called a Directive will enhance the versatility of procedures, particularly in the process environment. These directives are instructions to the software or hardware to perform user-specified options at particular points in a procedure or method. Such options could conceivably include various calibration options, diagnostic facilities, alarms and warnings, and some of the set up options which, once they have been selected in the present package, are fixed for the entire duration of the experiment .

Planning for a package with these capabilities is under way.

2.11 REFERENCES

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2.12 GLOSSARY OF TERMINOLOGY

Table V

Terminology used in FlowTEK

Detector	e.g., uv/vis spectrophotometer, ion-selective electrode, atomic-absorption spectrophotometer, etc.
Device	e.g., pump, injection valve, switch, auto sampler, etc.
Method	Series of device events, event times, and instrument set-up options which together result in a single measurement.
Peak parameters	Peak height, area, width at a certain height, time of peak maximum, and concentration
Reduced data	Date and time of a measurement, peak parameters, method file name, and profile file name
Procedure	A combination of methods, other procedures, and WAIT steps
Profile	Plot of detector response versus time for the duration of a measurement
Configuration	A set of user-selected options
Auto zero	The process of subtracting a constant from all data points. The constant is measured at some point during the experiment (usually at the beginning) and corresponds to the detector response in the absence of analyte
Event	A change in the status of a device