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DESIGN CONSIDERATIONS IN COMPUTERISED THERMAL ANALYSIS SYSTEMS

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ABSTRACT

A new computer system has recently been introduced by Stanton Redcroft for the automatic control, recording and processing of thermal analysis experiments. Great care has been taken to integrate instrumentation and programming to optimise the benefits of this system. Various electronic and software design features are therefore discussed in order to show the importance of linking equipment design to the specific requirements of thermal methods.

INTRODUCTION

The ideal computerised thermal analyser would probably be a fast, accurate, versatile,easily operable system giving well presented results of exactly, the required nature and format. Practical considerations however require that we consider factors such as complexity, instrumentation and programming costs, as well as frequency and generality of use. It is obvious that individual requirements will vary greatly. We must therefore allow suitable (and sufficient) options within the various instrumentation. There are for example still many thermal analysts whose needs can be adequately met by a combination of equipment attached to chart recorders. We should therefore be careful not to neglect or lower standards in the thermal analysis instrumentation simply because we can manipulate data by computer to make it appear more acceptable.

In considering an integrated computer system it is convenient to separate the computer instrumentation (hardware) and the programming (software). The following sections specifically relate these two areas to thermal analysis and also to the design of the new Stanton Redcroft system.

INSTRUMENTATION OUTLINE (HARDWARE)

A general schematic outline for integrated computerised thermal analysis is given in Fig.1. The typical current nature of the various optional components are also indicated.although outward appearances will vary markedly.

Consider the 4 main areas as outlined:

1) Data input and instrument control

Generally, the sensors used in thermal analysers generate analogue (i.e. continuous) signals. It is therefore necessary to convert these signals into a form recognisable by the computer i.e. we must amplify (if necessary) and digitise. We should also electrically isolate the inputs from the computer system to prevent variable interactions (such as earth loops). Ideally all thermal outputs should be continually monitored to be certain of valid [illegible]

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e.g. temperature excursions may occur during thermal events which distort the preset thermal profile. Conversion from analogue to digital format by definition precludes continuous sampling. We can however approach the ideal by attaching a 'converter' to each input (rather than switching a single 'converter' between the two or more inputs). Whichever system is used, it is essential that it be capable of sampling sufficiently fast to give an accurate description of the 'most rapid meaningful change' applicable to the specific input type.[1]

Many experiments include both small and large thermal events. Computer systems are particularly useful for monitoring such extremes, since it is relatively easy to construct an interface with a larger dynamic range than a typical chart recorder. Analogue to digital (A/D) converters are normally used for this although even these devices have limitations to their resolution which may be exceeded experimentally. We have therefore found it preferable (since high resolution is important) to use individual voltage to frequency (V/F) converters, with a resolution of 1 part in 10^6.

It is important that dedicated computer systems are versatile and interactive, so as to allow the application of user expertise. An alpha-numeric keyboard is therefore necessary as this also allows the input of written information (although both standard and complex analytical methods may be loaded directly from disk).

2) Data manipulation

The basic computer requirements for thermal analysis are similar to those of many scientific applications. It is important to realise however that a maths processor can be a useful 'extra' for the many complex arithmetic operations likely. The system should be capable of being easily programmable by the user to allow for specific individual and research applications. The main requirement however, as with all other parts of the system is reliability, without which the benefits of high technology cannot be exploited!

3) Data storage

Thermal analyses generally contain periods where no significant thermal changes occur. If therefore we quantify this 'significance' and also the nature of the required result(s) we can truncate the stored data without any significant loss of detail.[1] In achieving this however it is particularly important to control the nature and frequency of the input so that high frequency and regular noise is minimised for each individual sensor type.

Collected data is normally stored within the dynamic memory (RAM) prior to analysis. The system must therefore contain sufficient memory (typically > 128K) for both the data and the programme, and should be expandable.

After analysis and output data may be stored for future reference. This is achieved by including within the system a semi-permanent storage facility such as 'floppy' or 'hard' disks. The choice of storage facilities (as on the Stanton Redcroft system) should really be defined by the user since it will depend on the size of the information store and the access speed required.

4) Data display

Experience of computer-analysed thermal data has shown that good screen resolution can be important when making decisions about subsequent data treatment. It is particularly important where single analyses include both large and small thermal events, in order to resolve detail. Colour resolution is also advisable, particularly for curve comparison. For general use, a 4 colour display with a 600 by 400 resolution is probably acceptable. The current Stanton Redcroft system displays 8 colours with a resolution greater than 700 by 500.

Similar resolution criteria should be applied to the selection of the device used for copying. This is normally a colour plotter but where a high proportion of written or tabular results are required, a printer is a useful optional extra. The selection of a graphics plotter is relatively easy in terms of resolution, colour, cost, and availability. It is therefore feasible to offer options both of size (A3, A4) and facilities such as chart drive.

PROGRAMME OUTLINE (SOFTWARE)

High level language programming is important in scientific software development as it reduces specific hardware dependence. Assuming therefore that the system is provided with a suitable operating system and a high level language (e.g. Basic, Pascal) the thermal software can be divided as indicated below.

5) Primary software requirements

Much of the overall programming involves basic data handling routines (such as data transfer, screen displays, plotting, error trapping, editing, choice selection etc.). Useful thermal analysis programmes however must include simple data manipulation functions such as curve scaling and comparison, differentiation, data storage and linearisation, basic peak and curve displacement analyses (peak time/temperature, weight change, area, extrapolated onset/offset) etc. It is important that the accessibility and operation of these routines are not compromised by the more complex functions. These 'simple' analytical methods should depend on the user specifying (either numerically or by cursor) the beginning and end of an event. This has been found to minimise manual and processing errors.

6) Special software functions

One important advantage of computer systems is that more complex experimental control and data treatments (e.g. purity, specific heat, kinetic determinations), can be routinely applied, due to the speed of operation. The added ability to link, and name complex temperature/gas change profiles and processing sequences however, should also prove invaluable in expanding the future use of thermal methods. The intelligent application of these methods implies certain important requirements i.e. good documentation (specifying the exact method), and the ability to add, modify, and replace functions. An absence of these features would severely limit the usefulness of a system for specific quality control and research applications. It is particularly important that well defined existing methods[2] can be implemented so that published data can be easily understood and compared. There is in fact a strong case for the standardisation of even the simplest processes (such as peak marking, extrapolated onset/offset). Certainly some indication of construction should be indicated to avoid confusion.

CONCLUSION

The design of computerised thermal analysis systems must, as indicated, take into account the specific requirements imposed by the nature and required accuracy of the thermal technique(s) involved. Provided that a suitable basic hardware design and correctly structured programming (using a high level language) is employed, future hardware and software development is relatively simple. The inclusion of these factors in the new Stanton Redcroft system allows for long term design stability whilst catering for future scientific advances.

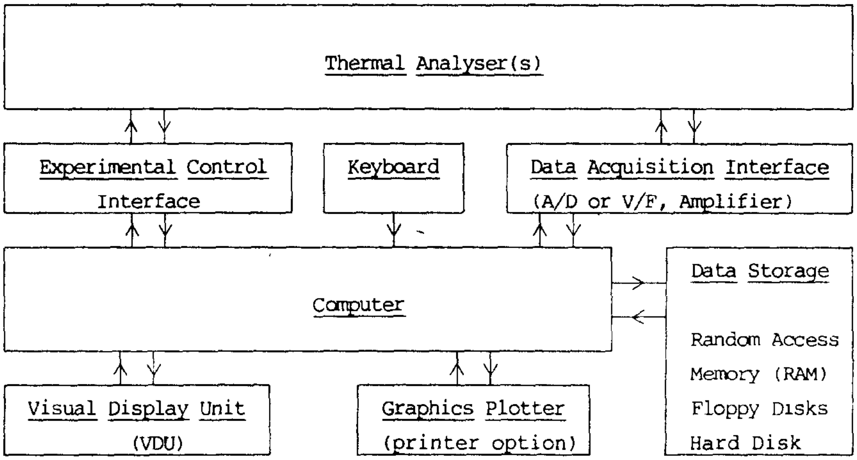

Fig.1 General schematic diagram for computerised thermal analysers.

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1 N.J.Manning, Anal. Proc. 21 (1984) 95

2 1984 Annual book of ASTM Standards, Section 14, Vol. 14.02. ASTM, Philedelphia 1984