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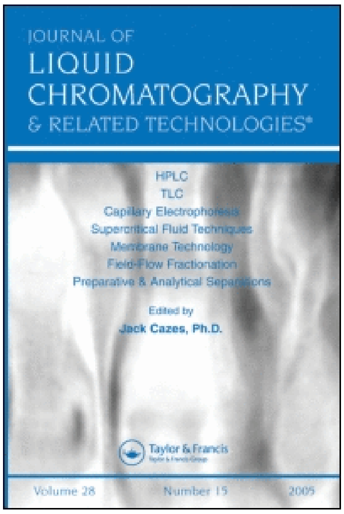

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Computers in Quantitative TL-Chromatography

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COMPUTERS IN QUANTITATIVE TL-CHROMATOGRAPHY

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ABSTRACT

The paper presents a discussion of the use of computers, mainly of the micro-processor variety, in devices for the photometric quantitation of TL-chromatograms. First a brief survey is given of the principal features of contemporary photometers specifically designed for chromatographic applications. The most sophisticated and expensive of these are dual wavelength instruments and at the present state of development only these have as yet been computerized. It is, however, anticipated that in the near future the use of computers will spread also to the less sophisticated single wavelength devices with a moderate price tag. The advantages are ease of operation as well as superior performance characteristics. The former is achieved using a computer to control the internal operation of the photometer and some of the possibilities open in this regard are discussed. The improvement in performance is achieved in a different way. Photometric quantitation of TL chromotograms requires a number of mathematical operations upon the signal on its path between the light source and the output display. The computer permits the use of almost any kind of signal transforms, transforms which would be completely impractical to carry out by traditional techniques. The acquired and preprocessed signal, which in a conventional device would be directly fed to the output recorder, can be subjected to "after-processing" with a substantial further gain in performance. The results obtained by computerized analysis are available in alpha-numerical form. Both hard and soft copy devices can be used. If desired a graphical display in analog form can also be obtained. The output information provided by the computer can be stored in extremely compact form on magnetic tape or disc with very fast access and retrieval.

INTRODUCTION

In today's analytical thin layer chromatography the ability to perform quantitative determinations is of almost equal impor-

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tance as the ability to separate itself. Of the various approaches to this purpose optical methods are widely preferred. The considerations of this paper apply specifically only to this approach to quantitative analysis. With appropriate modifications, however, many of the principles discussed are applicable also to other related methods of quantitation, not only of TL-chromatograms, but also to liquid (mainly HP) and gas chromatography.

With the growing interest in the optical quantitation of chromatographic separations the number of special purpose devices developed for this purpose has equally increased. They range today from relatively simple and inexpensive instruments for low to moderate performance to extremely sophisticated (and correspondingly costly) systems for the highest demands. (1) In the latest instruments of this class automation usually coupled with computer control is widely exploited. "After"-processing of the raw acquired data by an external or built-in computer is capable of improving the performance characteristics of the system further by perhaps an additional order of magnitude. But computer hardware has become almost ridiculously inexpensive. The main portion of the cost is on the software side, that is in the development of suitable programs and algorithms. Once this has been achieved and sufficient experience been collected, there seems to be no obstacle to the introduction of computerized control and processing also to less sophisticated and costly equipment. In these devices automation and data processing will probably be kept at a lower level of sophistication; nonetheless a considerable pay-off in terms of performance and operating comfort can almost with certainty be anticipated.

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Classification of Optical Methods of Quantitation

Optical (or photometric) methods for quantitative chromatography can by and large be divided into two classes, which may be labelled "densitometry" and "fluorometry". Both terms are here used in a broader sense than the common meaning of the words and some elaboration is, therefore, warranted.

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The term "densitometry" includes here both transmission densitometry (or "densitometry" in the narrower sense) and reflectometry. As a matter of fact the latter mode is used much more widely despite the theoretical superiority of transmittance measurements. The simple reason for that is the relatively high optical density of most standard separation layers especially in the UV. In consequence of this transmission densitometry is frequently not able to provide sufficient light to insure an adequate signal to noise ratio at the input of the electronic part of the system. (2)

The optical response of blank TL-media can be characterized by two basic parameters: the coefficients of absorption and scatter. For the application of optical methods of quantitation it is desirable, that the values of both coefficients show as little point to point fluctuation over the whole active area of the chromatogram as possible. Also their mean spatial values ought to be clearly constant everywhere and exhibit little dependence upon the range of optical wavelengths. For the purposes envisaged here this range extends from the far red or near infrared at about 800 nm to the medium UV at perhaps 200 nm. There is a marked tendency towards broadening this range at both ends.

Generally it is assumed that the presence of separated (and the case given suitably dyed) substance affects only the coefficient of absorption, but not that of scatter. (3) The optical response of the medium (the term covering both transmittance and reflectance) depends, however, on both parameters in a complicated way. As a general rule the presence of separated material can only increase absorption and consequently reduce the optical output. The essence of densitometric quantitations in chromatography is, therefore, the determination of the change in optical response of the medium in zone areas compared to blank regions. Using suitable mathematical transforms (frequently based upon empirical data), the increment in absorption causing the measured response change is derived and from the latter the underlying concentration.

The principal difference between densitometry and fluorometry is, that in the latter the illuminating radiation serves only to excite the examined material to emit secondary radiation at a somewhat longer wave length than the original. The big advantage of fluorometry is, that ideally areas of the chromatogram not containing separated substances appear black and the base line of the recording ought, therefore, to be perfectly flat. In practice this is, of course, only partially the case. An other advantage is that the optical output changes linearly with concentration.(4) This is in marked contrast to the generally high non-linear relationship between these two parameters in densitometry.

For many substances fluorescence has to be induced by coupling to a strongly fluorescing agent. In many respects this procedure can be likened to the staining commonly required for densitometry.

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A number of other methods exist which employ, directly or indirectly, optical radiation for the detection and/or quantitation of material analyzed by chromatographic or related procedures. Significant as many of them are, they usually serve specialized narrow purposes and use special purpose equipment, which frequently has few features in common with the more general purpose photometric quantifiers which are the subject of this discussion. Acknowledging the existence of these devices may, therefore, suffice for the present purpose, leaving them to the specialized literature of the fields they serve.

There is also a number of devices in use, which employ different kinds of non-optical radiation. Many of the arguments used in the context of this paper for optical measurements can be extended to these as well. Space does, however, not permit to consider these cases and the modifications they require in any detail.

Classification of Photometric Devices

Commercially available photometric equipment for application in chromatography can be roughly divided into single wave length and dual wave length devices. (5),(6)

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Single wave length devices represent the vast majority of all photometers in current use. This design can be kept simple and their cost is, therefore, relatively moderate. Their performance is adequate for most routine application. Generally they are designed as multimode instruments, which can be used in any of the modes of operation discussed in the preceeding paragraph.

As already indicated by the name, single wave length devices employ a single near monochromatic beam of light to scan the surface of the analyzed chromatogram. The spectral width and position of the beam is usually adjustable using filters or a monochromator. When used for fluorescence measurements, better instruments permit independent adjustment of the spectral position of the exciting beam and of the measuring beam. Modern requirements call for a very wide spectral range which cannot be covered by a single light source. It is then customary to employ two suitable light sources, one for the long and one for the short end of the spectrum. The intensity of illumination ought to be kept as stable as possible. It must be adjustable to match the optical characteristics of different media.

Most single wave length devices work with a slit shaped aperture. The length of the aperture slit is usually adjustable to match chromatograms with different track widths. A slit shaped aperture yields a signal which is proportional to the mean light intensity over the length of the slit. But due to the generally non-linear relationship between concentration encountered and the light intensity received, a slit shaped aperture can yield markedly erroneous results unless the concentration profile along the slit is kept closely constant. This does not apply to fluorescence, the intensity of which is a closely linear function of concentration. To obtain the total amount of substance in a zone, the concentration values obtained from each slit position have to be added (integrated). But to find the concentration value even within a single aperture field, the response characteristic has to be first linearized in terms of concentration. Simpler instruments employ to this purpose an empirically obtained sequence of calibration points. More sophisticated devices use mathematical transforms mostly implemented electrically by analog circuits. (7) The final integration over the whole zone area is usually performed manually from the recording strip, where results of the analysis are displayed.

The performance of any measuring method is ultimately limited by noise. Photometric methods for chromatography are essentially affected by two types of noise. One is of electrical origin and can be reduced almost arbitrarily by adopting a sufficiently high intensity of illumination and by choosing low noise electronic components. The other and usually decisive component is optical noise. The intensity of the optical noise component is largely determined by the optical homogenity of the separating medium. Little can be done to improve it further in single wave length devices.

Far reaching compensation of the optical noise component is the main raison d'être of dual wave length instruments. It should, however, be noted, that this advantage applies only to a relatively small degree, when the instrument is used in the fluorescence mode.

Dual wave length scanners have also a number of other though less significant advantages. When the two beam signals are combined by ratio forming, not by subtraction, intensity fluctuations of the light source are largely eliminated. Instruments of this kind usually employ instead of a fixed slit aperture a flying spot scanning system. This feature abolishes the necessity to keep the transversal concentration profile constant and gives thus greater freedom in the application of the sample. (1)

The main drawbacks of dual wavelength photometers are complexity, higher demands upon the skill of the operator and concurrently high cost. Dual wavelength operation is, however, the method of choice when the ultimate in performance is required and investment costs come second. Computer processing of the acquired data can further considerably improve performance and the resulting cost increment is not that high in proportion to the basic

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price. It is, therefore, not surprising that dual wavelength photometers were the first ones to be considered for teaming up with a computer and later for integrated computer design.

The Role of the Computer

The potential of computer processing in TL-chromatography had been recognized at a fairly early date. One of the first papers in this regard is probably a report by the present author presented at a symposium in Philadelphia in 1971 and later published in print. (8),(9) At that time, computers powerful enough to handle even the basic requirements of the chromatographer were bulky and expensive. Few workers in the field of chromatography had then even an elementary understanding of the principles of programming and signal processing. The concept of signal to noise ratio as the basic limitation for performance was also relatively new in this area, though it had already proven its power in many other disciplines. It is thus no surprise that for many years little practical progress was made.

The turning point came with the advent of the micro-processor and associated break-throughs in the technology of large scale integrated electronics. A contemporary micro-processor based device with the same data handling capabilities as a minicomputer of 1970 costs a fraction of the price of the latter even in today's inflated dollars. Power requirements, size and weight were also drastically reduced. Permanent instruction sets are routinely stored in low cost "read-only" (ROM) memories with large storage capacity. Transition from one set of instructions to another can be made by simply replacing one preprogrammed ROM unit by another one. Fundamental programming knowledge is today fairly widely spread; a significant advantage in this regard is, that even very small machines can today be programmed in one of the popular high level languages (Basic, Pascal, etc.), which enable an operator even with little computer experience to carry out some independent programming and adjustment of existing programs according to his individual needs.

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Other significant developments opening the road to a much wider application of computer technology were far reaching improvements and cost reduction of output devices both of the soft (picture tube, CRT) and hard copy (print) variety. Where archival quality is not required, the results obtained can also be stored semi-permanently on magnetic tape or disc. This makes file keeping and retrieval much easier and faster. Simple alphanumerical displays can for little extra cost be supplemented by graphic capabilities if necessary in color. The operator communicates with the machine usually via specially designed keyboards. Important progress was also made in many other aspects of computer technology, which here cannot be covered in any detail. Jointly all these advances were instrumental in triggering the so called, "Computer revolution", which is affecting all aspects of contemporary life.

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Microprocessors are today even incorporated into a vast variety of consumer products and professional devices. In the field of TL chromatography the inroads made are, however, still few and in between and there is ample room for more. The following pages will be devoted to a survey of what the present situation is and to the potential for future development.

TLC Analysis Systems With Integrated Microprocessor

Computers are today extensively used in conjunction with analysis systems of many kinds. Two approaches can here be distinguished. In the first, the older one, the computer together with a suitable interface for data transfer is simply added to the system. It usually operates upon the data, which would normally appear at the output of the analysis system and does not affect the internal operation of the latter. Its main purpose is the improvement of the quality of the obtained results and bringing them into a form, which is more convenient for perusal by the analyst.

In the second approach, which evolved later, the computer forms an integral part of the system. In addition to operating

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upon the output data of the system, it exerts control over most of its internal functions. A built-in computer is usually able to perform besides its function as a controller all the tasks of an add-on external processor; there seems to be, therefore, no need for a separate discussion of the latter alternative. The use of a micro-processor as integral part of the photometer has become economically attractive and technically feasible as a direct consequent of the technological progress discussed before. In most cases the "brain" of the system will be a micro-processor. The relatively slow processing speed of these devices compared to that of a mini-computer is in applications of this kind usually no obstacle. The use of an "intelligent" controller, as micro-processor equipped devices are frequently dubbed, permits to achieve an otherwise unobtainable degree of automation and performance. In this context it may be worth mentioning, that microprocessors are intended primarily for logical decision making and for numerical computations only in the second place.

The Control Functions of the Built-in Computer

In its function as a controller the built-in microprocessor provides signals which initiate, supervise and terminate virtually all phases of a particular analysis operation. To this purpose the processor has to receive on a continuous basis all data, which are relevant for the transition from one operational step to the next one. It must also dispose of a set of logical equations (a program), into which the data available to the machine at any given moment are inserted as variables. With these data the program equations provide unambiguous instructions for the next step of the operational sequence. In present systems it is inevitably assumed, that the available data are adequate to arrive at such a decision. In the few exceptional situations where this may not be the case the program is arranged so as to call for operator assistance. It is quite probable that in the future alternate modes of decision making will be adopted, where the decision logics need not be completely specified in advance by the programmer, but where it is gradually established and refined through a "learning" process, which utilizes past experience stored in the memory of the machine.

The form in which the electronic and electro-mechanical subunits of the system are able to generate data and to receive instructions may differ considerably from the form in which the central processor accepts or transmits these data. "Interfacing" the heterogeneous parts of the overall system becomes then a key problem, which may not always be easy to solve.

Consider now the individual features which might be subject to microprocessor control. For briefness only dual wavelength devices will be discussed. Virtually all operations which might be suitable for automation in a single beam device are needed also by double beam instruments. By simply omitting features not required by the former, the discussion which follows can immediately be applied to both types.

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The topic is perhaps best covered by following the operational routine of a typical device. Details may, of course, differ for different models. After fitting the chromatogram to be analyzed to the support table and switching on power, the operator may key in the spectral windows for the two beams or, in a more sophisticated arrangement, simply specify the substances he is looking for and the development procedures used. The pertinent spectral data would in this case be retrieved from memory. In either case the machine takes then care of the adjustment of the position and, where necessary, of the width of the monochromator slits or of the positioning of the filter wheels.

The next step is the adjustment of the illuminating intensity for both beams to obtain the best obtainable balance and a convenient light amplitude at the photodetector input, in the case of photomultipliers, without danger of overload. (10)

Further magnitudes to be keyed in are the transversal and longitudinal scanning velocity, the useful widths of the scan and the number of tracks on the chromatogram. The processor converts then the received numerical instructions into the corresponding setting of the control elements for the respective operation. For optimum results it is also desirable to change the electrical bandwidths of the electronic circuits to conform with the chosen scanning velocity. Execution of the keyed in instructions is confirmed by displaying the set values on the display and usually also on the hard copy print out. To shorten the analysis time the machine can be instructed to use a higher scanning speed over blank portions of the medium and return to the desired operating values only when a zone area is discovered.

Another parameter which can be automatically controlled is the sensitivity and/or measuring range. The range setting is automatically taken into account during the subsequent mathematical operations and may appear on the print out or graphical output.

The machine can also be instructed to advance automatically from one track to the next one. It is desireable to use for the return to the origin a higher speed then the one used for scanning. In many designs this is difficult to achieve. A simple expedient is then to simply reverse the direction of the scan. Since the data can be kept in memory and the sequence reversed before being displayed, the reversal of the scan direction does not appear on the output graphs. When the desired number of tracks has been scanned, the system switches itself automatically off and a signal to this regard appears at the operators command console.

The list of automatically controlled functions quoted above is certainly not complete; it is intended only as an illustration of the tasks a built-in processor is able to perform. In most cases the operator will have the ability to override automatic instructions.

Mathematical Operations

Automatic control of the equipment of the type described in the preceeding paragraph is merely a convenience, though a valuable

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one. It helps to speed up operations and reduces the demands upon the skill of the operating personnel. The main contribution of the built-in computer is, however, its ability to perform complex mathematical operations upon the signal, operations which frequently may be difficult if not impossible to carry out by conventional analog circuitry. Manual after-processing of the required data is in most cases too time consuming and cumbersome to be a realistic alternative. But the ability to perform these operations may be a prerequisite for a further substantial improvement of the performance parameters of the system.

The mathematical operations involved can be divided into two classes: Operations which are best performed on-line during the course of signal acquisition and those which can without significant detriment be performed off-line, i.e. when the basic information for the analysis has already been acquired. A built-in integrated processor, if properly dimensioned, is usually able to perform both functions on-line in addition to the supervisory and control functions mentioned in the previous paragraph. An add-on machine is usually suitable only for off-line or true "after"-processing. Since the costs involved in both approaches do not significantly differ, the built-in alternative seems to be almost always preferable. This applies even when an already existing computer is available for after-processing. The reason for this seeming paradox is the relatively high cost of intermediate data storage and interfacing equipment together with the expenses for the necessary software, which in these cases may have to be custom developed.

The most important results of quantitative TL-analysis is the amount of separated substance contained in a given zone. To obtain this magnitude the coefficient of extinction of the analyzed substance(s) must be known. In a computerized device this value can frequently be fetched from memory, where it had been stored during a previous run. Otherwise routine calibration procedures have to be followed, the results of which are then transferred to memory.

To obtain the total amount of substance in a zone the measured changes of the optical response of the medium in zone areas (compared to blank portions of the chomotogram) have to be integrated over the width of the zone. With slit scanning devices only one step of integration, in the longitudinal direction, is required. Flying spot devices require two steps of integration: One transversally and one longitudinally.

Integration is equivalent to addition. Addition is, however, feasible only, if the system response is linear in terms of concentration. With fluorometry this is almost always the case and no special steps towards linearization are needed. The situation is quite different for densitometry. The optical response of the photometer is almost always a highly non-linear function of concentration. Before integration (or summation) can take place, the output of the device has to be linearized with respect to concentration. Relatively simple mathematical transforms for this purpose were derived by the author. (11) These transforms can be implemented by analog circuits or digitally. In the latter case it may sometimes be preferable to use empirically determined look-up tables in conjunction with an interpolation algorithm. Either way digital transformations can be made much more accurate and stable with time.

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The transform values are then added point by point in the central processor until the boundaries of the zone are reached. Criteria for determining this can vary from simple threshold settings to fairly sophisticated curve fitting and interpolation procedures. These criteria were, of course, already decided upon during the software development for the system.

When integration over a zone area is completed the data are shifted into storage and kept there for later use, e.g. for printout and/or display. Sometimes it may be desireable to store the results obtained together with supportive information required for later identification on magnetic tape or disk; from these storage media the results can be retrieved by automatic search procedures.

Magnetic storage of information is extremely compact and retrieval is fast and easy. It has, however, to be kept in mind that these storage media are not suitable for very long term preservation with archival quality.

Processing may be stopped after integration and the obtained results are then usually displayed on a CRT screen for print-out together with the necessary auxiliary information. Formatting of the print-out and the support data is usually already established by the basic program. However, the operator may type in any additional information he feels desireable to be retained. The built-in keyboard which serves for all communication between the system and its environment can be used also for this purpose.

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After-processing

The results available at this stage can be considerably improved by further processing the data which would normally represent the output information. The following options, individually or jointly, are available for this purpose. Other procedures may become available as development proceeds and further experiences are gathered. An attractive feature of this technique is, that the performance of the system can be substantially improved for little additional cost. The computer hardware necessary for process control and the basic mathematical transforms is usually capable of handling the requirements of after-processing without much expansion. The cost involved is, therefore, largely restricted to the cost of the necessary software only. The first and possibly the most significant step in after-processing is the establishment of a smooth synthetic base line. This reduces vastly the influence of random fluctuations of the optical response of the blank medium (optical noise) which is the main factor contributing to base line noise. But the effect of fluctuations due to electrical noise is also strongly diminished. The base line may also show systematic trends reflecting non-random changes of the optical transfer of the medium. These are usually the consequence of non-uniform development and/or drying. Base line shifts of this kind can frequently be abolished or at least reduced by suitably modifying these procedures.

Base line noise is usually reduced (complete elimination is even theoretically not possible) by some kind of smoothing algorithm, e.g. by mean square interpolation or filtering. Systematic base line changes require a different approach. However, if the chromatogram has been properly processed these become noticeable only at the highest sensitivity settings.

Base line smoothing improves the accuracy of the results obtained since the amplitude of the signal obtained from zone areas is always measured with respect to the base line as zero level.

In dual wave length devices optical base line noise is almost completely compensated; electrical noise remains then as the principal source of base line noise. (It should be noted that electrical noise is not reduced by the dual wavelength principle, but on the contrary slightly increased.) The situation is different when a zone of separated substance is encountered. Here even with dual wavelength scanning and under ideal conditions some residual optical noise remains. With adequate design and properly chosen operating conditions the total noise encountered in zone areas is almost exclusively determined by the optical component. It can be substantially reduced by after-processing employing similar techniques as those used for the compensation of base line noise. In both cases the noise content of the signal is reduced by minimizing the random deviations of the measured signal from an idealized curve, the character of which has been established before hand, the exact position of which is, however, not known. An underlying assumption is that the medium is macroscopically homogeneous along the whole length of the chromotogram, an assumption which with todays commercial media is mostly justified.

For base line compensation the curve to be minimized is a straight line. In the absence of systematic trends it is also known that this line has zero slope. For the compensation of

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zone noise the idealized contour is curvilinear. Basically two approaches are available. The first one specifies only, that the contour be smooth. Mathematically this can be achieved by using the so called "spline" functions usually of the third order. The second technique assumes that the concentration profile within the zone follows piece-wise a Gaussian curve; the parameter σ^2, which is the main characteristicum of a Gaussian function, may have different values at the leading and at the trailing edge of the zone. If the sample has been applied in line form at the origin, the iso-concentration curves are approximately straight lines perpendicular to the axis of the chromatogram. When spotting is used, the iso-concentration curves become approximately semi-circular or semi-elliptical (11). The spline technique requires more computational effort, but has the advantage that the zone contours are obtained almost automatically. The second approach is easier to implement, especially if the iso-concentration lines can be assumed to be approximately parallel straight line or concentric circles; there seems to be little difference in the accuracy of both methods.

Once base line and concentration profile of zone areas have been smoothed and the signal amplitudes within the latter determined by subtracting the smoothed zone signal from the interpolated base line, integration can be carried out using any one of the standard procedures for numerical integration. The simplest of these is probably straight summation of the sample values using a staircase approximation to the smoothed concentration profile. The width of the individual step is then determined from the spacing between samples which in turn ought to be approximately equal to the width of the scanning aperture. In most situations a degree of overlap between adjacent scan elements is encountered, which has to be corrected before or after integration. The latter method requires less computational effort.

Displays

When processing is completed, the results obtained have to be returned for final interpretation to the operator. The computer output are clearly digital data. It can in this form be displayed on a CRT screen; an associated printer is usually desired to provide a "hard copy" version of the output which is demanded in most cases. Usually both numerical data and explanatory verbal text are provided; the latter may partly be printed under program control, with the rest being keyed in manually by the operator, who decides also (within limits) the format of the displayed message.

The choice of data to be outputted is completely flexible. Data displayed under program control may typically comprise the characteristic data of each zone, e.g. position of the peak, the integral of the optical response, calibration constants, the integral of concentration, range setting, monochromator adjustment, date and perhaps time of the day of analysis etc. The information typed in for display by the operator may contain data specifying the proceduresused like solvent system, development technique, origin of the sample and its quantity, a code symbol for the operator and/or analyst etc.; when an automated system for filing and retrieval is used, the operator may also have to key in the appropriate file code and identification number. Besides the paper print-out storage of the output data on magnetic tape or disc may also be desireable. Magnetic storage is extremely compact and lends itself to fast retrieval by an automated system. However as already remarked before, magnetic storage media have only a limited retention time for the stored information and are, therefore, not suitable for archival purposes.

Chromatographers so far have been accustomed to a graphical output in the form of a curve displaying concentration with respect to distance from the origin. Display techniques of this kind are usually labelled "analog" as opposed to the above mentioned digital format. Though digital presentation is more precise and in most cases more informative, many chromatographers will find a conventional analog recording useful. To this purpose it becomes necessary to convert for each scanning line the optical response or concentration value supplied by the computer in numer-

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ical form, to an "analog" voltage value. The converted data can be regarded as equidistantly placed samples of a conventional recording. They can be recorded by a point printer or joined into a continuous curve using low pass filtering, linear interpolation or another suitable technique. The curve can be viewed on a storage oscilloscope, if hard copy output is not requested.

Plotting devices with direct numerical control by the computer are also available, but fairly expensive. For the purpose envisaged the approach described above appears to be more economic and to yield satisfactory results.

Many current analog recorders can be fitted with an alphanumerical printing device as accessory. Digitally controlled devices can also be instructed to write alpha-numerical characters under program control. Either technique permits to retain also on the analog recording some of the numerical and verbal information available on the digital print-out.

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CONCLUSION

The built-in computer offers almost unlimited flexibility in design and operation. The aspects of computer control and processing in the field of quantitative photometry for TL-chromatography, which are discussed in this paper, should therefore in no way be regarded as exhaustive and covering the whole area. On the contrary the intention has been only to illustrate the possibilities which exist for the use of computers in this field and the advantages which can be expected from this approach. With progress advancing at the present rate new features and applications will certainly evolve in the near future. It can also be anticipated that the use of computers will fairly rapidly spread from the most sophisticated devices in the highest price class, which are at present its exclusive domaine, to the simpler and less expensive instruments used in everyday's laboratory practice.

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