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Wavelength control and spectrophotometric analysis using personal computer

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ABSTRACT

Spectrophotometer is an analytical instrument used in research and industry to characterize the materials. In this, the transmission or reflection of the sample is measured as a function of wavelength. The main objective of the paper is to convert the analog single beam UV-Visible manually operated Spectrophotometer into a wavelength control and spectrophotometric analysis (automatic) using personal computer. A software package was also developed for the wavelength selection in the 340-960 nm ranges and for the evaluation of Transmittance/Absorbance/Concentration of any chemical substance. With this modification there was a tremendous reduction in the time required for the qualitative and quantitative analysis. Printing of the absorption spectrum and identification of the absorbance peaks of any given sample was also made possible with this computerized instrument. The performance of this modified instrument was evaluated using the standard annular grade samples. In this modified instrument high resolution grating monochromatic, high sensitive photodiode (for entire spectral range) and high speed wavelength scanning. The results are well comparable with the standard values. The paper deals with hardware and software.

KEYWORDS

Wavelength;
Spectrophotometric analysis;
Personal computer.

INTRODUCTION

Spectrophotometer is a venerable instrument in science and technology. Fraunhofer used it to investigate the composition of the sun. It has been used to investigate molecular structure of the chemical solution. Spectrophotometry is one of the widely applied physicochemical techniques, which is remarkable for its sensitivity and precision[1]. Substances in solutions possess the property of absorbing light, at specific wavelength, characteristic of the particular substance. This basic principle of absorption is utilized in the measurement of various concentrations[2]. The spectrophotometer is one such instrument which has varied applications ranging from research to routine jobs like the estimation of protein content in the blood, nucleic acid molecules, detection of soil organic compounds, determination of enzymatic activities on organic matter etc. Several attempts have been made for wavelength control and spectrophotometric analysis[3-4]. However, these have conventional and they have their limitations. In the present study, we convert the analog single beam UV-Visible manually operated spectrophotometer (Model CL-27) into an automatic wavelength control and spec

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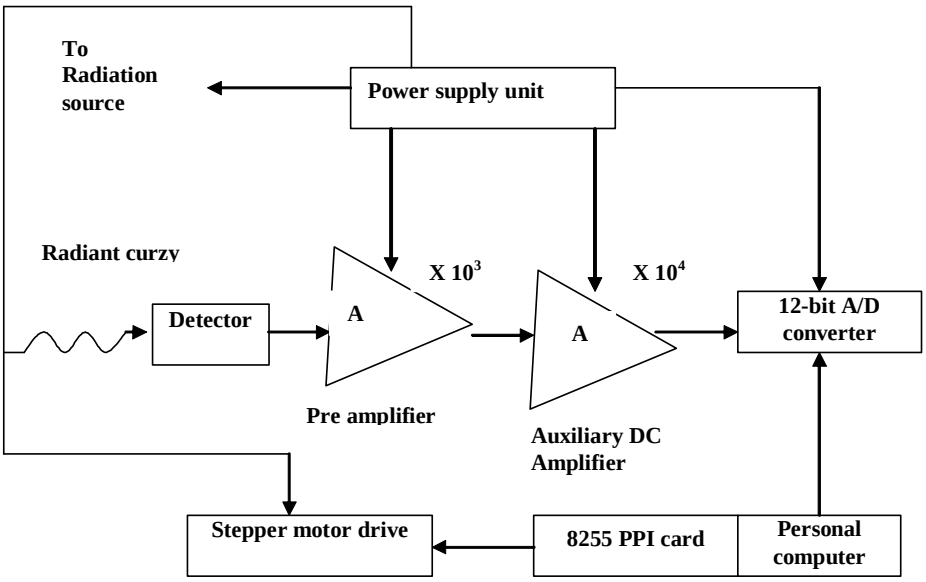


Figure 1: Block diagram of computer-based spectrophotometer

Figure 2: The photograph of gear wheel mechanism of computer based spectrophotometer

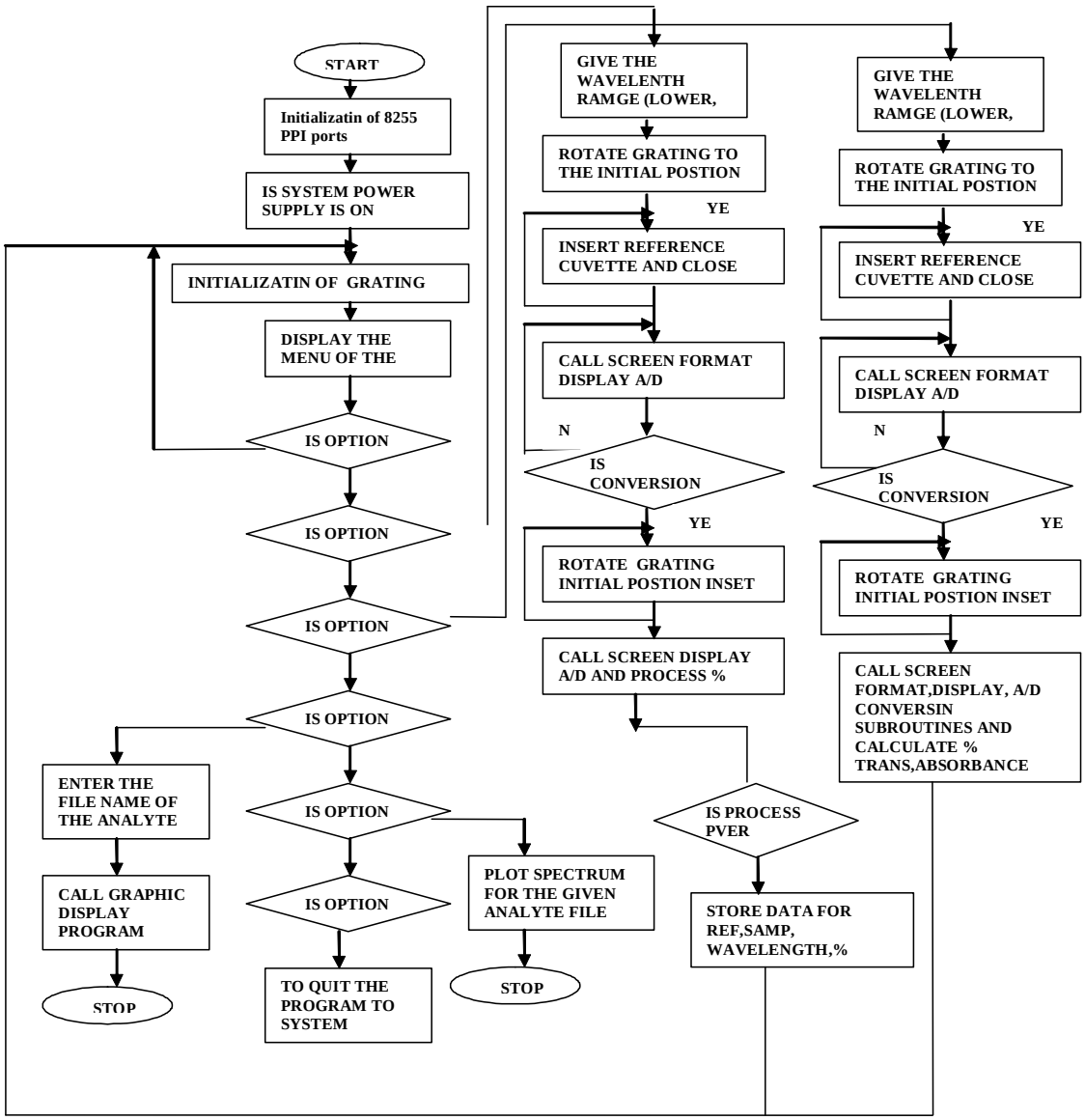
Figure 3: The photograph of complete computer based spectrophotometer

trophotometric analysis using personal computer. The advent of microcomputers has opened up the new possibilities in the area of instrumentation for wavelength control and spectrophotometric analysis.

Instrumentation

Hardware design

The block diagram of single beam UV-Visible (Model CL 27) manually operated spectrophotometer into an automatic wavelength control and spectrophotometric analysis using personal computer is shown in figure 1. The single beam spectrophotometer constructed with the components of a radiant source of a Tungsten filament lamp, a Dispersion element of grating with 600 lines/mm, a sample curette for inserting the samples and radiation detector. The output of this radiation detector is fed to a data presentation system. The manual wavelength selection (grating rotation) is replaced by incorporating a stepper motor[5] Gear Wheel mechanism. The previous wavelength selection of 5nm of each step in unmodified instrument is increased precisely to 1.5nm by coupling a larger gear wheel of diameter of 13.5cm having 253 teeth which was attached to the shaft of the grating mount and a small gear wheel of diameter 1.35cm having 23 teeth was coupled to the shaft of the stepper motor. This provides an 11:1 reduction in the angular rotation of the grating mount. The stepper motor was operated at 200 steps per revolution so that 8 revolutions of stepper motor were required to convert the wavelength range of 620nm i.e. from 340 to 960nm. Hence total 1600 steps were required to convert this range. The Gear Wheel mechanism arranged with the Stepper motor and Grating provided a precision of 0.375nm for each step. The photograph of stepper



Flowchart of system software

Figure 4: Flow chart for a computer based spectrophotometer

motor Gear wheel mechanism and the complete system of computer based Spectrophotometer is presented in figure 2 and figure 3 respectively.

The interface between the stepper motor and the additional hardware with computer was achieved by insetting a Digital Input Output Timer (DIOT) and add-on card for PC/XT/AT compatible systems developed by Electro System Associates (ESA) Bangalore is used in the present instrument[6]. In the manual operated system the radiation detector output was given to pre amplifier circuit with OPA128[7] with highly stable temperature characteristics. This offered high input impedance and provided an output maximum of about 600mv. But ICL 7109[8](12 bit A/D converter) incorporated by the author in the modified Spectrophotometer requires a minimum of 2v as reference voltage. Hence an auxiliary DC amplifier was also incorporated to amplify the output of the preamplifier to about 2v. The auxiliary DC amplifier was designed with IC3140 in non-inverting configuration. The ICL 7109 is a monolithic 12-bit A/D converter designed for easy interfacing. It has 14 three state outputs, 12 data bits, 1 polarity bit and 1over range bit. These bits are enabled either by the CE/LOAD, LBEN and HBEN control signals or by entering the handshake mode. It can be controlled through I/O peripheral ports such as 8255 PPI

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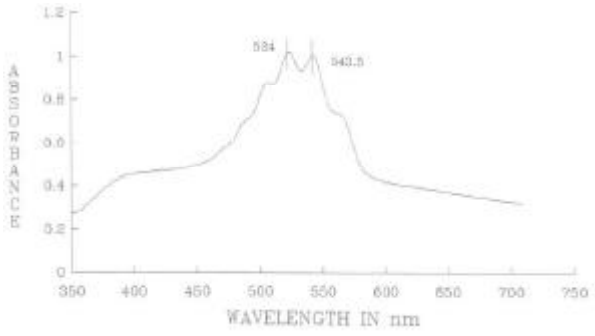
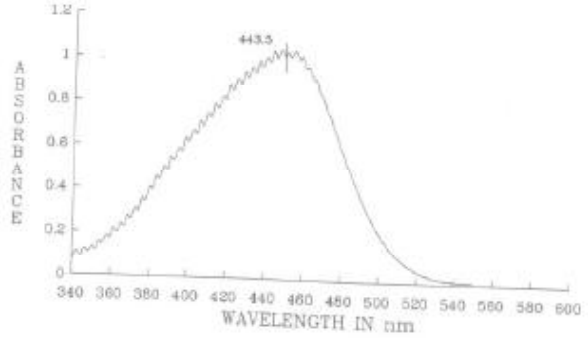
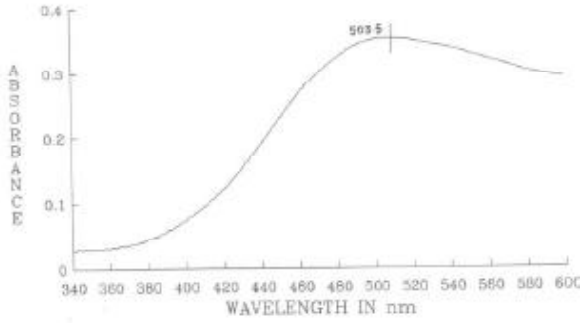


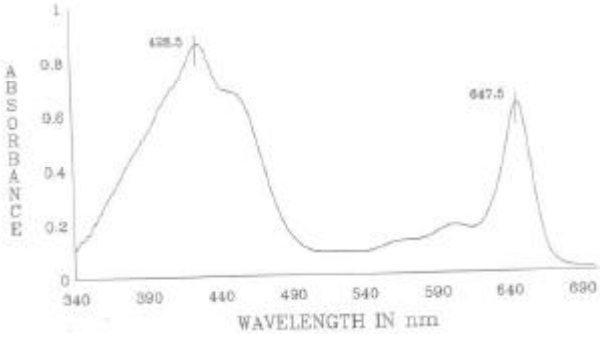
(a): Absorption spectrum of potassium permanganate



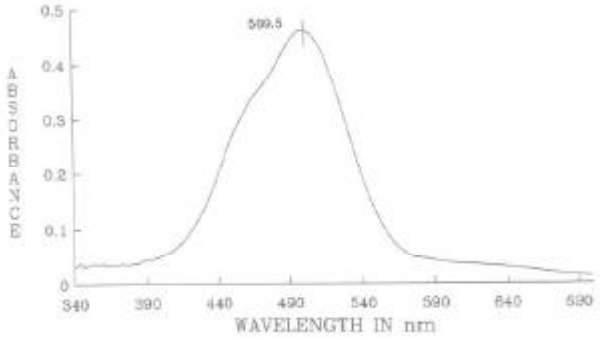
(b): Absorption spectrum of potassium dichromate



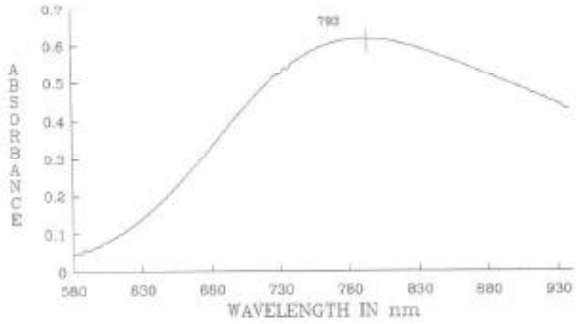
(c): Absorption spectrum of manganese



(d): Absorption spectrum of chlorophyll



(e): Absorption spectrum of cobalt chloride



(f): Absorption spectrum of copper sulphate

Figure 5: The absorption spectrums for some samples using computer based spectrophotometer

card is straight forward interface circuit with microcomputer for the absorbance measurements. The features are a true differential input, the ability to measure both positive and negative input voltage and an on-chip reference voltage generator. An input of +1v will generate the same 12 bit data, as an input of -1v. However, the POL pin will be at logic high for positive input and at logic low for negative input. When the RUN/HOLD input is tied high, the ICL7109 continuously performs analog to digital conversions. The STATUS pin indicated the end of conversion.

Software

The necessary software for the operation of the system is developed in C language[9]. The main role of the software in the present study is to govern the user to carry out the Spectrophotometer analysis of the given sample solutions in estimating the parameters such as % Transmittance and Absorbance in the wavelength range of 34-960nm. The following functions are to be carried out precisely and accurately.

1. To rotate the grating of the spectrophotometer precisely with a stepping motor by generating appropriate pulse signals in sequence.
2. To enable the data acquisition system to convert the

TABLE 1 : Maximum peak absorption

S.no	Analyte	Maximum peak absorption (nm)	
		Present study	Literature value
1	Potassium permanganate	526, 547	525, 545
2	Chlorophyll	428.5, 647.5	420-430, 645
3	Cobalt Chloride	509.5	510-515
4	Potassium dichromate	443.5	440
5	Manganese	493	500
6	Copper sulphate	800	810

analog information into digital information.

3. To set the position of the grating according to the desired wavelength range required by the user.
4. To scan for the wavelength corresponding to the absorption peak of the given analyte.
5. To compute and display the data of the analyte and graphically represent its spectrum.
6. To make different functional units of the system work in a proper sequential order.
7. To indicate defects of the hardware if any.

The flow chart of the program is presented in figure

4. The necessary software for the operation of the sys tem is developed in C language.

RESULTS AND DISCUSSION

The performance of this modified instrument was evaluated using the standard samples of annular Grade Chemicals. Spectrophotometric analysis was carried out individually for each analyte adopting the procedure cited in flow chart. The software program developed by the author enabled to identify the wavelengths corresponding to the absorption maximum values. This package also facilitated the absorbance wavelength characteristics and % transmittance wavelength characteristics with maximum peak absorption. The results are presented in TABLE 1 and its corresponding spectrums are shown in figure 5.

CONCLUSION

The hardware and software features of single beam UV-Visible manually operated spectrophotometer (Model CL-27) into an automatic with wavelength control and spectrophotometric analysis using Personal Computer are described. The necessary software is developed in C language. The modified system is more accurate then the previous system. In the present study, high speed wavelength scanning through the computer controlled drive system accurate measurement of wavelengths corresponding to absorbance peaks in the instrument's wavelength range of 340-960nm with an accuracy $\pm$ 0.2%, the same optical path is used for both reference and sample solutions. Nearly constant energy is present throughout the wavelength range of 340-960nm and rapid recording of entire spectrum and the real time data acquisition and processing through an IBM PC and graphical display of the absorption characteristics. The conversion of single beam UV-Visible manually operated spectrophotometer into an automatic wavelength control and spectrophotometric analysis using personal computer is a special feature of the present study.

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