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THE APPLICATION OF A SMALL DIGITAL COMPUTER
TO THE CONTROL OF A MASS SPECTROMETER*†

C. R. Lagergren and J. J. Stoffels

Battelle Memorial Institute
Pacific Northwest Laboratory
Richland, Washington 99352

INTRODUCTION

The decision to use a computer to operate our mass spectrometer came as a result of the frustrations we felt at having to rebuild or modify repeatedly the instrument components responsible for automatic operation. Automation of some kind is usually required in order that the data taking process may yield a maximum of useful information. For example, in thermal emission mass spectrometers, used for isotopic abundance measurements, the ion emission rate varies with time. To compensate for this variation a time symmetric scheme of sampling the isotopic constituents of the ion beam is devised. One such scheme, most commonly used, is to produce alternately forward the reverse scanned spectra on a strip chart recorder. This requires a circuit capable of varying either the magnetic field or the ion accelerating potential in the triangular manner with time. When ion counting methods are employed to measure ion beam intensities, some device which will produce a time-symmetric step function in one of the fields is used. Additional requirements on the design of the device used in this case include provisions for independently selectable sampling times and a variable number of sampling steps. Also provision must be made for the necessary delay times required for stabilization of the ion beam following each step. Our experience has been that we were never sufficiently clever in designing the degree of flexibility into an automatic system that would include the improved scheme of taking data suggested by operating experience. The best approach to the design of the

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ultimate system seemed to be one in which a small digital computer could be made to control the magnetic and electric fields of the mass spectrometer. Also, digital output of our ion-counting detector is in a form inherently suited as a computer input. Then as new and improved operating modes are desired it is necessary only to modify the operating programs (software) rather than rebuild control circuits.

Although our primary motive in developing a computer controlled system was to achieve versatility in automatic operation of the mass spectrometer, three other beneficial factors were considered. First, the computational ability of the computer offers on the spot reduction of data in its final form. Proper detailed calculations that one would never have time to do manually could be accomplished. Second, the overall sample handling capacity of the instrument could be increased to the ultimate limitation imposed by the mass spectrometer itself. Third, a variety of data output forms such as a printed report, punched paper tape, and IBM cards could be produced automatically and magnetic tape systems could be used to facilitate data storage and retrieval operation.

DESCRIPTION OF THE SYSTEM

(Slide 1 - Artists sketch of mass spectrometer and block diagram of control system.)

The first slide shows the basic arrangements of control. The top half of the slide is an artists conception of the fundamental elements of our mass spectrometer. It happens to be a thermal emission instrument having three analyzer stages, two magnetic stages in a zero dispersion configuration followed by an electrostatic analyzer. The basic reason for this arrangement is to obtain an abundance sensitivity in the parts per billion range--which it does. That is, in the uranium mass region the tail of the major isotopic ion-beam component at its adjacent mass positions is reduced to a few parts per billion of the major beam intensity. The mass resolution corresponding to the slit widths used is about 1 in 400.

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Material loaded on the sample filament is thermally ionized, accelerated to about 14 kilovolts of kinetic energy, and focused into a beam issuing from Slit S_1 . The red and blue areas represent two separated isotopic components of the ion-beam, the red being the more massive. Mass selection occurs at Slit S_2 between the two magnetic analyzers. Permanent magnets having gap field intensities of about 8500 gauss are used. They are matched in field strength by mechanical shunts not represented in this picture. Controlled variations in gap fields are produced by coils wound around the analyzer vacuum housing in the central planes of the gaps. Current in these coils is furnished by a power supply which is controlled through the interface by the computer. The Slit S_3 is located at the zero dispersion point of the combined analyzer system. The potentials of the electrostatic analyzer plates as well as the ion accelerating potential are provided by a single high voltage power supply which is also controlled through the interface by the computer. The function of the second magnetic and the electrostatic analyzers is to remove those ions of the wrong mass which by some scattering process succeed in passing through Slit S_2 . The "clean-up" action of these stages increases the abundance sensitivity about four or five orders of magnitude. Beyond the exit Slit S_4 of the electrostatic analyzer the ion-beam is accelerated an additional 40 kilovolts in energy into an aluminum target. Secondary electrons, represented here in green, are accelerated by the 40 kilovolt field into a plastic scintillator. The light pulses produced in the scintillator are sensed by a photomultiplier which in turn puts out a pulse for each ion passing through Slit S_4 . This is a version of the ion detector developed by Dr. Norman Daly of Aldermaston, England.

The lower half of the slide shows the control system. The "heart" of the system is the computer which is a PDP-5 (now obsolete) made by the Digital Equipment Corporation. It has a memory of 4096 12-bit words and is equipped with instruction skip, program interrupt, and data break features as well as an 11 bit analog to digital conversion unit (Type 137). The interface, shown as the annular box surrounding the computer, is rather complicated to describe in detail. Basically it contains a number of codable device selectors, device condition flags, input and output buffer

registers, a precision digital to analog converter, a data break multiplexer, a relay multiplexer, and a crystal clock.

Control of the magnetic field is accomplished as follows. A binary number corresponding to the field strength desired is transferred from the accumulator of the computer to a 12-bit output buffer. The voltage analog of the number contained in the buffer is used as the reference voltage for the internal regulating circuit of the magnet sweep current power supply. Control of the ion accelerating voltage is accomplished in a similar manner except that the output buffer for this device sets relays which change the feedback resistance of the supply's internal regulating circuit.

Pulses from the anode of the photomultiplier are fed directly to a gated discriminator whose output drives a 24-bit scaler input register of the interface. The first 3 bits of this register are contained in a high speed prescaler. The overall dead time of the ion counting system is set at 41.5 nanoseconds to insure against faulty operation. Gating of the discriminator is under control of a crystal clock and a 12-bit scaler register. Gate times in multiples of 1/880 seconds up to 4096 units or about 4.65 seconds are available.

The ADC unit shown next to the discriminator is a Nuclear Data pulse height to digital converter which through the data break multiplexer utilizes 256 words of the computer's memory to form a pulse height analyzer. It is thereby possible to test or monitor the performance of the ion detector and set the discriminator threshold to its proper condition.

At the bottom of the interface box are shown a number of analog inputs which can be selected via the relay multiplexer for conversion by the computer's ADC unit. It is possible, although we are not currently using but one of these inputs, to monitor under program control various conditions such as analyzer and source chamber pressures, filament current or temperature, etc. The one input we do use is a variable voltage from a 10-turn helipot which can be programmed to set or vary in a continuous fashion either of the power supply output buffers. This removes the frustration of trying to think in binary while making

essentially continuous changes in control parameters. The relay multiplexer also provides for several output functions. Currently the only one used is to set the polarity of the magnet sweep current although a variety of servo-mechanisms could be operated to perform other control functions such as turning equipment on or off or adjusting source focus controls.

At the lower left are shown several input-output devices. The oscilloscope display permits a wide variety of information to be observed visually. Some examples will be shown later. The teletype keyboard and printer is the main communication link between the operator and the system. Operating programs are written so as to receive coded commands from the keyboard and in some cases the computer interrogates the operator via the printer. Two magnetic tape units are used: One to provide rapid loading of the operating programs into the computer and the other to store raw data from each analysis. 4096 words of memory is not sufficient to hold simultaneously all of the programs needed for control, data reduction, output, and storage. The paper tape reader is used primarily as a backup system for loading the computer in the event that something goes wrong with the magnetic tape system. An IBM key punch has also been interfaced to the computer which allows us to output data on IBM cards.

(Slide #2 - Photograph of complete instrument.)

The second slide is a photograph of the entire instrument with the exception of the key punch which happens to be located out in the hall. On the right is the 3-stage mass spectrometer mounted on an "L-shaped" slab of granite. The ion source is located in the metal block which has the bundle of white wires connected to it. The first magnet is just behind the source block and the second magnet is to the far right. The electrostatic analyzer is housed in the 90 degree pipe elbow in front of the second magnet. The control system is to the left. The first blue cabinet behind the teletype contains the magnetic tape units, the second the PDP-5 computer, and the third most of the interface circuitry. The other racks contain power supplies, vacuum gages, and various control circuits.

(Slide #3 - Mass Spectrometer only.)

The next slide is a closer view of the mass spectrometer taken at about the same perspective as the artists view in the first slide. The trapezoidal-shaped object near the magnet yoke is the field shunt used to match the two magnetic fields. The end of the magnet sweep coil can be seen. The brass can houses the photomultiplier.

(Slide #4 - Closeup of sweep coil.) ✓

The next slide shows the sweep coil with the magnet rolled back. The coil is cast into a lucite form which is fastened to the analyzer tube. The 80 turns are wound up the front edge, loop over the end, down the back, and loop over the other end. Half of the turns loop over and half under the tube at the ends so that their axial fields cancel in the vicinity of the ion-beam.

EXAMPLES OF OPERATION UNDER COMPUTER CONTROL

The computer programs currently in use with the mass spectrometer can be categorized as adjustment or testing, data collection and processing, and data storage and retrieval routines.

(Slide #5 - Part A of printed report.) ✓

Slide #5 is an example of the kind of report that is produced by the data collection and processing program used for a uranium isotopic analysis. The computer requests information as to sample identity and instrument operating parameters by typing out the headings that appear in the first five lines to the left of and including the colon. The operator responds by typing in the requested information. The quantity "background" is the ion detector noise rate in counts per second. The deadtime is in units of nanoseconds. At this point the operator "tunes-up" the mass spectrometer and then returns control to the computer. This control program proceeds as follows. Mass positions 238, 236, 235, 234, then 234, 235, 236, and 238 are sampled in that order. Gate times for each increment are 1/2 second at 238, 4 seconds each at 236 and 234, and 2 seconds at 235. A delay of 1/2 second is used following each change to insure complete stabilization. At the bottom of the page total gate times per scan of 1, 8, 4, and 8 seconds for the respective mass are shown. One forward and

reverse scan or one cycle takes 25 seconds. At the conclusion of a cycle, while the next one is in progress, the computer types out the sums of the ion counts received in each mass sampling. You will note that the ion-beam intensity slowly decreased. When the intensity reached approximately two thirds of its initial value, the operator instructed the computer to halt at the end of the current cycle by a coded keyboard command. He then "retuned" the mass spectrometer and increased the sample filament temperature until the initial ion emission rate was reached. Control was then returned to the computer. After eight more scans the analysis was interrupted again. The decay rate during the third block of data suggested that the sample was nearly expended, so the operator issued the command to halt the analysis and proceed with the calculations.

(Slide #6 - Part B of printed report.)

The next slide shows the first set of calculations performed by the computer. Listed are the deadtime and background corrected ratios 236 to 238, 235 to 238, and 234 and 238 for each scan. Ratios 234 to 235 and 236 to 235 were also calculated but not printed. The calculations are all performed in binary floating-point and are outputted here as decimal floating-point numbers. The negative numbers in the first column are the result of subtracting a background rate from a zero count. The purpose in outputting these calculations is to give the operator an opportunity to examine the data for gross errors before the final results are obtained. He is instructed to eliminate any blocks of data which show significant trends or any lines in which the ratios fail the standard statistical gross error test. In this case when the computer asked which lines were to be deleted, the operator typed a "period" meaning no deletions. The total raw counts for each isotope and the number of complete sweeps used after editing is then outputted.

(Slide #7 - Part C of printed report.)

The next slide shows the output of final calculations. At the top is listed the average ratios from the previous table together with the corresponding variances, standard deviations of means, inverts of the averages, and standard deviations of the inverts. The 4/5 and 6/5 average ratios now appear also. The only other possible ratio remaining, the 234 to 236, is not determined. Just below the table of ratios

appears the isotopic composition of the sample in atom percents together with standard errors. You will recognize this as being a sample of natural uranium.

After reporting the average 238 deadtime and background corrected count rate during the analysis, the computer asks for its next command. The response "rite" means store the raw data and sample history on magnetic tape. The computer did so and reported where the data is located on the magnetic tape. The next two commands "data" and "calu" cause IBM cards to be punched. The parallel listing here is for varification purposes only.

The operator then called for another program which calculates the atom ratios and atom percents from the total counts received at each mass. The previous method of calculation gave equal weight to each scan. If the amount of data contained in each scan varies appreciably, that method would not be appropriate to use. In this instance, however, the second calculation routine was called in order to compare the total variability of the run to that caused by counting statistics alone. A comparison here of the errors associated with the 234 and 235 atom percents for the two methods indicates that the mass spectrometer did not contribute any significant variability to this analysis.

(Slide #8 - A mass spectrum.)

The next slide illustrates another type of control program, one in which a mass spectrum is produced. The mass range 237 to 243 is divided into 63 equal increments which are scanned in both directions counting ions for 1/2 second at each step. A 1/10 second stabilizing time is used between each step. The numbers of ions counted are accumulated for each mass increment in 63 corresponding locations of computer memory. The contents of these memory locations are continuously displayed on the oscilloscope screen using either logarithmic or linear scale factors. This is a linear display of a plutonium spectrum. The sample happens to be from a reactor physics fuel burnup experiment. The isotopic masses are from left to right 238, 239, 240, 241, and 242.

(Slide #9 - Peak shape display.)

One of the most useful programs for testing the alignment of the mass spectrometer is the peak shape display program. In it the ion-beam is swept rapidly in sawtooth fashion and the ion-counts observed in small sweep increments are plotted on the oscilloscope screen. Slide #9 is an example of the use of this program which illustrates a critical test of how well the sweep fields of the two magnets are matched. For this test Slit S_2 , the mass selecting slit, is set at its normal width of 0.023 inches. Slit S_3 at the zero dispersion point is adjusted to .004 inch and accurately centered on the ion-optic axis. The slide is a triple exposure of three test conditions. The horizontal scale is .001 inch per minor division. The first exposure was taken with the magnets scanning the peak at one extreme of the sweep range. The magnet sweep was then shifted and the high voltage changed accordingly so that the peak was scanned at the other end of the sweep range. The two peaks so obtained are almost exactly superimposed. The third exposure was taken after moving Slit S_3 .003 inch. The result clearly demonstrates the effect that would have been observed if, over the entire range of the magnetic sweeping system about .360 inches, the two fields failed to track so as to cause as much as a .003 inch net dispersion instead of zero.

(Slide #10 - Pulse height distribution.)

The last slide illustrates another test program that is used routinely to check the setting of the discriminator threshold of the ion counting system. Ion pulse amplitudes are digitized by the Nuclear Data ADC unit. The digital equivalent of the pulse amplitude becomes an address of computer memory which is incremented through the data break facility. The program is essentially one in which the contents of the ADC addressable block of memory are displayed. The result is a pulse height distribution of those pulses which lie above the discriminator threshold level. The threshold is adjusted so as to contain nearly the entire distribution due to ions and reject noise.

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