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COMPUTER CONTROL AND DATA PROCESSING FOR FIFTEEN ISOTOPE RATIO MASS SPECTROMETERS

C. Sulfridge

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OAK RIDGE GASEOUS DIFFUSION PLANT
OAK RIDGE, TENNESSEE

*prepared for the U.S. ATOMIC ENERGY COMMISSION
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Oak Ridge Gaseous Diffusion Plant
Union Carbide Corporation
Oak Ridge, Tennessee

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ABSTRACT

A small computer system has been interfaced to 15 isotope ratio mass spectrometers which operate continuously. Performance of the system has been highly satisfactory since it was put in operation early in 1971, and has enabled more effective utilization of the spectrometers. The system includes a PDP-8/I computer with 8K core memory, a 32K disc, one digital ratiometer, an input teletype, and an output teletype. The system automatically times the analysis events for individual spectrometers, collects the analysis data, performs the necessary calculations, stores certain results, and prints all results on the output teletype.

The foreground/background concept of programming was used with the foreground priority program performing essential spectrometer timing and data acquisition. The background program, which is written in FOCAL, allows the analyst to communicate with the computer by selecting one of several options which represent the various functions the computer will perform.

This system was assembled and initially programmed by Tennecomp Systems Inc. from specifications provided by the Oak Ridge Gaseous Diffusion Plant Laboratory. System description, operation, and advantages are discussed.

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COMPUTER CONTROL AND DATA PROCESSING FOR
FIFTEEN ISOTOPE RATIO MASS SPECTROMETERS

INTRODUCTION

The uranium hexafluoride (UF_6) isotope ratio mass spectrometers at the Oak Ridge Gaseous Diffusion Plant (ORGDP) Laboratory were automated¹ beginning in 1958. An analyst attached two samples, one often a standard, to the inlet system of a spectrometer, purified the samples, and depressed a start button on the program control. The spectrometer then automatically proceeded through the 12-step, 13-minute cycle necessary to complete a determination.* A digital ratiometer and printer were adapted to read out, on paper tape, the isotopic ratio readings for each sample.

After the completion of each automatic determination, an isotopic ratio of ratios or an isotopic concentration was calculated on desk calculators from the data on the paper tape.

Since many thousand isotopic determinations are made each month in this laboratory, considerable analyst time was required to collect the data from the 15 spectrometers and make the necessary calculations.

Specifications were written for a computer system that would perform the data acquisition, make the necessary calculations, and be compatible with existing automation components and electrometers for 15 spectrometers.

In 1970 a system meeting these specifications was delivered to ORGDP by Tennecomp Systems Inc. The necessary cabling and spectrometer modifications were completed by Laboratory personnel. A block diagram of the system is shown in figure 1.

Basic components of the system include a PDP-8/I computer with an 8K core memory, a 32K disc, a real time clock, separate input and output teleprinters, a Dana Model 5700 digital voltmeter (ratiometer), a Non-Linear Systems relay matrix, and a Tennecomp Autoloader.**

The spectrometer control interfacing is shown on the left side of figure 1. A single cable with four conductors connects each spectrometer to the control patch panel. One pair of conductors energizes a relay in the spectrometer program control panel which in turn energizes a stepping switch to advance the program a step at a time as determined by the computer program. The other pair of conductors is connected to a set of contacts on a relay in the program control which can be reset by the analyst. Closure of these contacts signals the computer that the spectrometer is ready to begin a determination cycle.

*A determination requires alternate introduction of two samples into the spectrometer with three introductions of sample 1 and two introductions of sample 2.

**These identifications are meant to be descriptive, rather than limiting. Other equipment with equal specifications may work equally well.

Figure 1
MASS SPECTROMETER COMPUTER SYSTEM COMPONENTS

The digital ratiometer interface is shown on the right side of figure 1.

Two electrometers in each spectrometer are coupled to the dual ion collection system. The output of the high-current amplifier (for the more abundant isotope) is automatically adjusted to about nine volts. The output of the other amplifier is determined by the concentration of the less abundant isotope of interest and the amplifier feedback resistor. These voltages are made to remain relatively constant, while determinations are being made, by automatic beam positioning and sample flow control devices within the spectrometer.

Each voltage from a spectrometer is carried in one overhead conduit up to 55 feet by a pair of wires within an aluminized Mylar shield and outer insulation. Two such pairs are carried within a third shield containing a very heavy *drain* wire and outer insulation.

Only the ratio of the lower voltage to the higher voltage for each spectrometer is required in the abundance determinations. Two relays in the relay matrix, under computer control, simultaneously couple the two voltages to the digital ratiometer; the higher voltage is coupled to the ratiometer reference input and the lower voltage to the ratiometer signal input.

The magnitude of the voltages allows a ratio range of approximately 0.01 to 0.09; thus, no range changing of the digital ratiometer is required. Six decimal places may be read from the ratiometer in this range.

The 32K disc holds over 6000, three-word variables plus the entire processor core image which can be recalled to the processor by depressing a single button on the autoloader. Since the system operates on an around-the-clock basis, heavy-duty teleprinters are used. The input teleprinter is used to converse with the computer, and the output teleprinter is used for data output under program control only. Figure 2 is a photograph of the computer system, with some of the spectrometers in sight.

SUMMARY

Experience with the system has been highly satisfactory. The number of determinations per analyst per hour has almost doubled since the computer installation, and the variance per determination has dropped from 2.5×10^{-8} to 1.6×10^{-8} . Some of these gains are attributed to improvement in the spectrometers themselves; however, they have been implemented through use of the computer system. Although the ratiometers and printers have been retained on each spectrometer as backup equipment, maintenance of these components is now negligible. Maintenance experience with the computer system for two years ending in February 1973 showed < 0.5% down-time.

The system is accomplishing the job it was designed for, but greater flexibility could be realized with additional storage capacity.

Figure 2

COMPUTER SYSTEM WITH SOME OF THE ATTACHED SPECTROMETERS

SYSTEM PROGRAM

The system program requires ten isotopic ratios to be read for each introduction of a sample. The averages for the readings on each sample are used in the computation of the ratio of isotopic ratios.

The foreground/background concept of programming was used with the foreground priority program performing essential spectrometer timing, data acquisition, and preliminary data manipulation. A priority real time clock interrupt occurs three times per second, and the relay scanner is advanced to connect to the next spectrometer; thus, the cycle time for 15 spectrometers is five seconds and a given spectrometer is serviced every five seconds.

The ready relay contacts on each spectrometer are sensed to determine which spectrometers have been activated by the analyst. If a spectrometer has been activated and a determination has been scheduled for that spectrometer by way of the background program, an action table is scanned to determine what action is to be taken on the particular spectrometer. The computer then either advances the spectrometer program control and begins a delay period, takes a voltage ratio reading, or ends the determination and performs preliminary calculations.

At the end of a determination, control is released to the background program for approximately two seconds for further computations, and the data are loaded into the output teleprinter buffer.

The background program, which is written in FOCAL,* allows the analyst to communicate with the computer by selecting one of several options which represent the various functions the computer will perform.

Three FOCAL program texts of 2000 words each are stored on the disc and a swapping routine automatically brings into core memory the FOCAL text with the routines necessary to process the requested option. A common group of instructions in each FOCAL text is used for computation and formatting of output data.

OPERATION OF SYSTEM

Operation of the system is initiated by the analyst identifying himself on the input teleprinter and then requesting 1 of 13 options currently available.

The input teleprinter response to a frequently used *schedule* option is shown in figure 3.

*FOCAL (FOrmula CALculator) is an on-line, conversational, interpretive computer language. FOCAL is a trademark of Digital Equipment Corporation, Maynard, Massachusetts.

ANALYST? 31
 OPTION? S
 SPEC? 8
 ENTRIES? 6

TYPE	R#	T#	P#	G#	S#
↑ <u>M</u>	↑ <u>4432</u>				
↑ <u>W</u>	↑ <u>4433</u>	↑ <u>490</u>	↑ <u>1</u>	↑ <u>2</u>	
↑ <u>W</u>	↑ <u>4434</u>	↑ <u>491</u>	↑ <u>2</u>	↑ <u>1</u>	
↑ <u>C</u>	↑ <u>4435</u>				
↑ <u>C</u>	↑ <u>4436</u>				
↑ <u>Z</u>	↑ <u>4437</u>				↑ <u>5134</u>

OLD R (T) = 1.092270
 NEW? NO
 OLD SV = 0.716460
 NEW? NO

ANALYST?

Figure 3
 INPUT TELEPRINTER COPY

Those items typed by the analyst are underlined. In this example, analyst 31 requested option S, to schedule a series of six determinations to be made on spectrometer 8. The determination type code tells the computer what type of computations are needed at the end of the determination and whether or not storage of the data on the disc is necessary. Only isotopic ratio, w, determinations are stored on the disc for later analysis of variance computations. Other information typed in by the analyst pertains to identification of the determination and factors, such as isotopic standard values, necessary in computation of results.

After an analyst sets up a schedule for a spectrometer, he must attach and prepare the samples on the spectrometer in the same order as they were scheduled. When the analyst depresses the reset button on the spectrometer, the determination is automatic through printout on the output teleprinter.

Options available to the analyst are shown in table 1. The abbreviations used by the analyst to initiate the options are shown in parenthesis.

Table 1
OPTIONAL FUNCTIONS

-
1.	(S) Schedule a spectrometer.
2.	(A) Abort a schedule of determinations.
3.	(R) Restart a spectrometer.
4.	(RR) Rerun a scheduled determination.
5.	(MI) Manually insert data on the disc.
6.	(C) List determinations with common identifications stored on the disc.
7.	(B) List spectrometer biases determined by computer.
8.	(I) Inventory the determinations made by an analyst.
9.	(RP) Print report of final averages of results stored on the disc.
10.	(TV) Analyze variance of a block of stored data.
11.	(T) Define a test.
12.	(CT) List accuracy verification.
13.	(Q) Halt background program.
-

Figure 4 shows a sample of output teleprinter copy. The first column is the determination type, the second column identifies the spectrometer on which it was run, the third column is the computed result, and the remaining data are scheduling and identification information.

M	4 =	1.02640,	655,	39	
M	6 =	1.01533,	85,	39	
M	7 =	1.02727,	2228,	39	
Z	2 =	3.027680,	13,	6375	39
W	12 =	1.01732,	574 (	491, 6, 1)	40
W	11 =	1.01929,	1648 (	491, 5, 1)	40
W	10 =	1.01736,	541 (	491, 3, 1)	40
W	9 =	1.01896,	1185 (	491, 4, 1)	40
W	8 =	1.01541,	39 (	491, 1, 2)	40
Z	1 =	0.583223,	616,	203	40
W	12 =	1.01723,	575 (	491, 6, 1)	40
W	11 =	1.01918,	1649 (	491, 5, 1)	40
W	10 =	1.01741,	542 (	491, 3, 1)	40
W	9 =	1.01887,	1186 (	491, 4, 1)	40
W	8 =	1.01541,	40 (	491, 1, 2)	40
W	13 =	1.01756,	3103 (	491, 7, 1)	39
C	3 =	1.092160,	1251	39	
C	4 =	1.017960,	656	39	
W	6 =	1.01909,	86 (	479, 14, 1)	39
W	7 =	1.01843,	2229 (	491, 8, 1)	39

Figure 4
OUTPUT TELEPRINTER COPY

The simplicity of FOCAL programming allows option operations to be easily changed to meet the needs of the operations with minimum downtime.

Changes in the foreground program, such as in delay times or the length of a determination, can be made relatively easily.

SYSTEM ACCURACY VERIFICATION

Since only one ratio measuring device is used, an error in the ratio determination could go undetected for a period of time before one of the control samples run daily would indicate trouble.

A system was installed on one of the spectrometers to allow a ratio to be set up on a precision decade from a stable voltage source. This ratio is read by the computer system during a test determination cycle.

Each digit from the digital ratiometer is presented to the computer accumulator in 1 - 2 - 4 - 8 binary coded decimal format. Numbers are set up on the precision decade to check each of the four coded lines for each digit during the determination. This determination is made daily and the results are monitored for possible errors in the system.

ACKNOWLEDGMENTS

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