N. P. Wilburn
L. D. Coffin

Combination of On-line Analysis with Collection of Multicomponent Spectra in an On-line Computer*

Abstract: A digital computer has been interfaced to four 256-channel analyzers. All functions of normal multichannel analyzers have been reproduced by suitable coding. In addition, a weighted least-squares method for estimating on line the contribution of individual radionuclides in a multicomponent pulse height spectrum has been incorporated. Details of the mathematics and coding methods, which include special modifications to an existing FORTRAN system for on-line use, are described.

Introduction

Early in 1964 a Containment Systems Experiment was undertaken by the Battelle Memorial Institute, Pacific Northwest Laboratories. The primary purpose of the CSE program is to evaluate, on a significant engineering scale, the effectiveness of natural processes and engineering safeguards in limiting the release of fission products from nuclear reactor accidents to the environs.[1,2] The secondary purpose is to investigate engineering aspects of a contained coolant loss accident, including the dynamic effects of a rupture in high-temperature coolant piping, and the leakage characteristics of representative containment systems. The program is directed to investigating the loss-of-coolant accidents in reactors of the pressurized or boiling water types.

A large number of radioactive samples of various kinds will be collected throughout this experimental program. Approximately one run will be made per month throughout the program. During the course of each of these runs, approximately 1500 radioactive samples will be collected. These samples will consist of filter assemblies containing four selective filters, bottles of liquid, and gaseous samples which will be collected and liquified in ampoules.[3] Each of these samples will be counted by means of a multichannel analyzer. Utilizing suitable calibrations, the isotopic concentration of the sample will be determined from the spectrum collected.

The Containment System Experimental Facility is located approximately 30 miles from the central data processing facility; hence there could be a rather lengthy turnaround between collection of the spectra and processing of the data by the central facility. This lengthy turnaround time has disadvantages. Foremost, if an error is made in the collection of the spectrum, there is no possibility of determining this fact until well after the analysis had been completed. Though most of the isotopes which would have been in the sample are relatively long half-life isotopes, the locating and recounting of the sample would cause a great deal of difficulty. Because of these reasons, a decision was made to purchase an on-line digital computer, and analog-to-pulse digital converters of a multichannel analyzer which would be connected by means of a hardware interface such that the memory of an on-line computer would be shared with the multichannel analyzer. This arrangement allows dual utilization for the memory unit, as well as the possibility of doing on-line computation with the data immediately after collection, using the central processor of the computer. With this system, all normal functions of a multichannel analyzer as normally sold by most manufacturers would be duplicated by means of programmed instructions to the computer. In addition, several analyzers could share the computer memory; and as was finally decided, four multichannel analyzers could be connected to the computer and operated simultaneoulsy. A PDP-7 computer manufactured by the Digital Equipment Corporation (DEC) was procured and interfaced to four Nuclear Data Corporation Type 180F analog-pulse-to-digital converters.

Description of hardware

The computer was basically the standard PDP-7 system which is supplied by Digital Equipment Corporation.[4] The details of the differences are as follows (a schematic block diagram is shown in Fig. 1):

1. Three magnetic tape units, the DEC tape (Type 555) dual transports, were included along with a DEC Type 34 oscilloscope display control unit.

*The work was done at Battelle Northwest, Richland, Washington

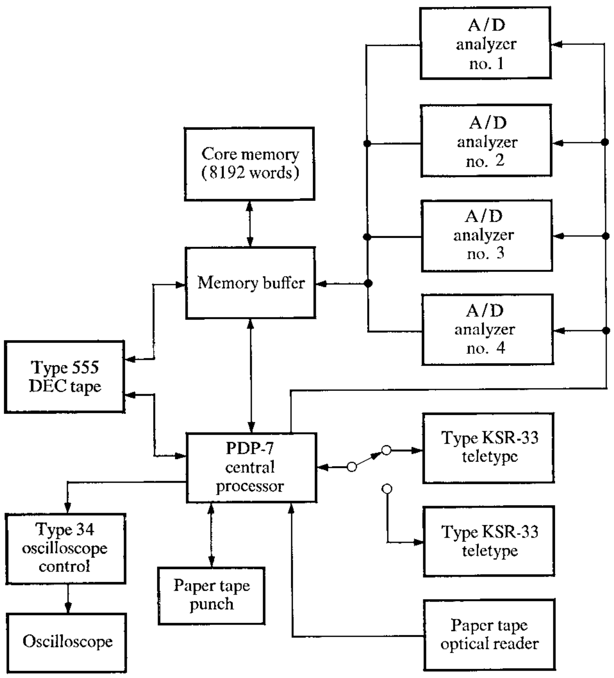


Figure 1 Block diagram of system hardware.

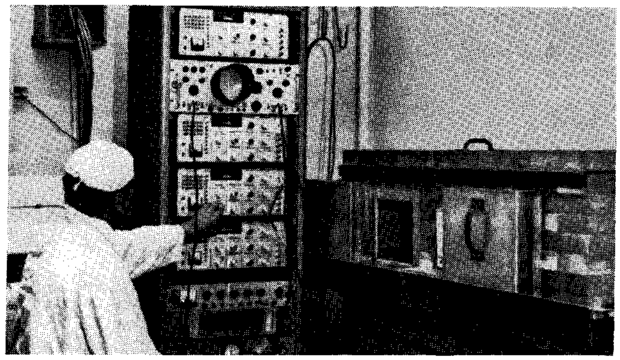


Figure 2 Counting room.

2. In order to allow simultaneous use of the computer's FORTRAN type programs, and interrupts from the magnetic tape units and from the multichannel analyzers, the EXTEND switch which was not used on this particular machine was changed in function. When the EXTEND switch was on, interrupts from the paper tape reader, punch, and teletype input-output unit were disabled.

3. Four Nuclear Data Type 180 F multichannel analyzer analog-to-digital converter units were interfaced to the computer utilizing the data break.[4]

4. When the analyzer has been enabled through an input-out transfer (IOT) instruction,[4] it continues operation until either it is disabled by means of another IOT instruction or an overflow occurs in any of the memory locations and turns off the analyzer simultaneoulsy.

Each one of the four multichannel analyzer inputs is connected to a phototube which is set in place in a separate lead-brick-lined cave (Fig. 2). Each one of these caves has four shelves which correspond to four different geometries used for the counting of a sample. As currently designed, the computer code will allow up to nine different types of samples at each of the four geometries, and eight isotopes for each of the four analyzers. The different sample types are required because a point source is not assumed for the sample being counted.

Mathematics of the spectrum analysis

The mathematical model used for the on-line quantitative analysis of individual radionuclides takes into account statistical variation in the gross sample spectrum and the errors associated with the counting instrument variabilities. The instrument variability is assumed to be a fixed percentage of gross counts and can be determined experimentally. In general, the modified weighted least-squares method which was used and the analysis described herein differs from classical methods in two ways: (1) The background spectrum is included in the model and estimated simultaneously with the other components and (2) the weights reflect instrument variability. For a detailed description of the probability model, see Refs. 5 and 6.

Two basic assumptions are made when using this model:

(1) The background count remains constant over n sampling periods on a given detector and (2) the group probabilities are known without error. Actually, the standard spectra counting error must be much less than any error associated with the unknown spectra.

If we denote the total count in the i^{th} channel group ($i = 1, N$ where $N_{\max} = 20$) for a given unknown spectrum, as Y_i and let y_{ai} be the total counts in the i^{th} group due specifically to decay of the a^{th} nuclide ($a = 1, k$; $k_{\max} = 8$), then $Y_i = \sum_{a=1}^{k} X_{ai} + B_i$ where B_i is the background for the group and the channel grouping is determined by instrument drift and the isotopes considered. We regard both X_{ai} and B_i as independent sets of chance variables and derive the model for the weighted least-squares analysis in the following way.

Let b_i be the background count rate in the i^{th} channel group. Denote the unknown sample live time interval by Δ and let C_a equal the estimated counts for the a^{th} nuclide during Δ time. g_{ai} is the channel group probability for the i^{th} channel and the a^{th} nuclide and $\sum_{i=1}^{n^*} g_{ai} = 1$ for

* This system allows up to 20 groups to be selected at operate time. However, they are normally fixed and are optimum for the particular set of isotopes expected in the sample.

$1 \le a \le 8$. g_{ai} is a conditional probability that a count is recorded in i^{th} channel group given that a single atom of the a^{th} nuclide decays. Then the model becomes $Y_i = \sum_{a=1}^{k} C_a g_{ai} + b_i\Delta + \epsilon_i$ where ϵ_i is the random error having mean zero. $C_a g_{ai}$ is the total count in the i^{th} channel group due specifically to the a^{th} nuclide.

We seek to minimize the weighted sum of squares, Q, with respect to the quantities C_a, where

$$Q = \sum_{i=1}^{n} \frac{\left(Y_i - \sum_{a=1}^{k} C_a g_{ai} - b_i\Delta\right)^2}{S_i^2}.$$

S_i^2 is the group weighting factor and is given below. The expressions resulting from the minimization are:

$$\sum_{a=1}^{k} C_a\left[\sum_{i=1}^{n} (g_{ai}g_{\beta i})/S_i^2\right] = \sum_{i=1}^{n} (Y_i - b_i\Delta)g_{\beta i}/S_i^2 \ ;$$

$$\beta = i, 2 \cdots k.$$

In matrix form the equations become:

$$\begin{bmatrix} \vdots & \\ \sum_{i=1}^{n} g_{ai}g_{i\beta}/S_i^2 & \cdots \\ \vdots & \end{bmatrix} \begin{bmatrix} C_1 \\ \vdots \\ C_k \end{bmatrix} = \begin{bmatrix} \vdots \\ \sum_{i=1}^{n} (Y_i - b_i\Delta)g_{\beta i}/S_i^2 \\ \vdots \end{bmatrix}$$

or in short notation:

$$[A]\vec{C} = \vec{D}$$

$$\vec{C} = [A]^{-1}\vec{D}.$$

The Crout method is used for the matrix inversion. The expression for the weighting factors is: $S_i^2 = Y_i + [\rho Y_i]^2 + \Delta^2 b_i/t + [\Delta\rho b_i]^2$ and is derived as follows:

Assuming a Poisson distribution,

$$\hat{\text{Var}}\ (C_a) \cong C_a. \tag{1}$$

By adding the relative instrument variability factor, ρ, we have:

$$\hat{\text{Var}}\ (Y_i) = Y_i + [\rho Y_i]^2 \quad \text{and} \tag{2}$$

$$\hat{\text{Var}}\ (b_i) = \text{Var}\,\frac{(C_i)}{t} = \frac{1}{t^2}\hat{\text{Var}}\ (C_i)$$

$$= \frac{1}{t^2}[C_i + (\rho C_i)^2]$$

or

$$\hat{\text{Var}}\ (b_i) = \frac{b_i}{t} + (\rho b_i)^2, \tag{3}$$

where t is the time associated with collection of the background spectra b_i. But we are interested in the variance of the term Δb_i where Δ is the sample live time interval, thus

$$\hat{\text{Var}}\ (\Delta b_i) = \Delta^2\frac{b_i}{t} + (\Delta\rho b_i)^2, \tag{4}$$

and adding (2) and (4) we have: (5)

$$S_i^2 = Y_i + (\rho Y_i)^2 + \Delta^2\frac{b_i}{t} + (\Delta\rho b_i)^2.$$

The relative standard error E_a gives some indication of the value of the estimate of C_a. $E_a = \sigma a/C_a$ (where σ_a^2 are diagonal elements of $[A]^{-1}$). The residuals of the group count estimates are given by: $r_i = (Y_i - \sum_{a=1}^{k} C_a g_{ai} - b_i\Delta)/S_i$. If the model is correct, the normalized χ_n^2 statistic should fall within the interval $[-3, 3]$, where

$$\chi^2 = \sum_{i=1}^{n} r_i^2 \ ; \qquad \chi_n^2 = \frac{\chi^2 - (n-k)}{\sqrt{2(n-k)}}. \tag{6}$$

(See page 22, Ref. (6) for the discussion on the degrees of freedom for method II.)

Generalized description of the multichannel analyzer code

Originally, it was hoped that the PDP-7 FORTRAN system,[8] with its possibility of inclusion of symbolic coding, could be used directly as a real time system because of the extensive mathematical manipulations that were necessary in the reduction of the analyzer data. However, the extreme difficulties encountered in using the FORTRAN system in this manner necessitated abandoning this procedure. Because of the extensive amount of coding already available in the FORTRAN operating time system (FOROTS) and the various software routines which operate the paper tape reader, punch, and teletype in FORTRAN codes, it was decided to retain use of the FOROTS system and to write the symbolic code much like that which would be generated by the FORTRAN compiler.

In the FOROTS system, as it exists in the magnetic tape DECSYS system,[9] there are numerous memory locations which are not required by the FOROTS when a program is completely operable. These areas can be used for scratch storage. For instance, there are a number of magnetic tape routines and debug routines which are incorporated into the FOROTS system. These are necessary during debug operations using the DECSYS system. In the design of the multichannel analyzer codes, these areas of memory were utilized for scratch storage.

In summary, all of the mathematical portions of the FORTRAN system, the .I01 Teletype input routine, the .I02 Teletype output routine, the .I03 paper tape reader routine, and the .I04 paper tape punch routine were used. The FORTRAN magnetic tape routines were not used because it was desired to operate the tape searches in a real time multiprogrammed sense[10] using the interrupt facility.

For purposes of description, the code may be divided into a "manual" portion and an "automatic" portion.

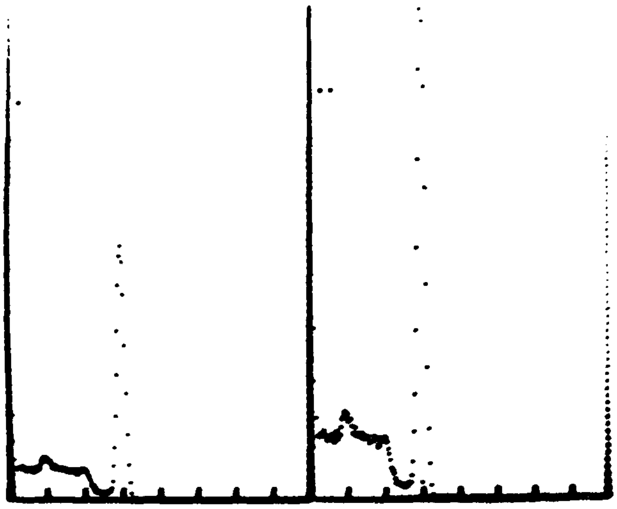


Figure 3 Typical dual analyzer display.

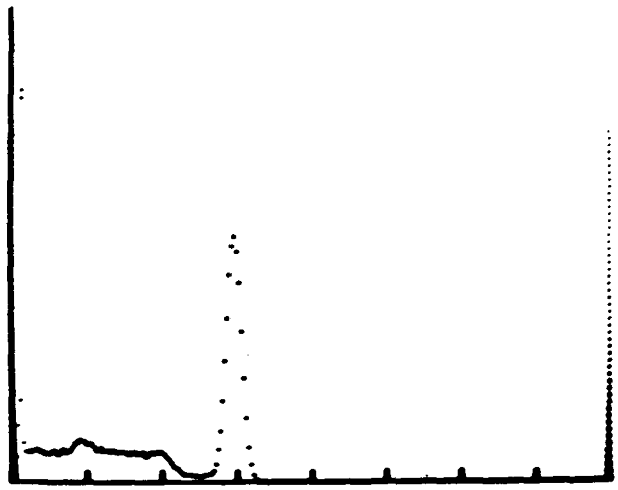


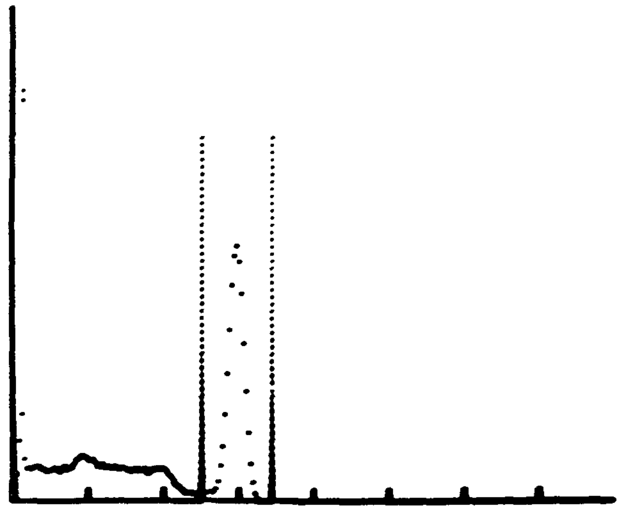
Figure 4 Typical single analyzer display.

The "manual" portion of the code contains the simulations of all of the operations which are normally available on a multichannel analyzer similar to those produced by Nuclear Data, RIDL, and so forth, plus some sections used for maintenance. By using suitable commands entered through the teletype keyboard, it is possible to turn the analyzers on or off, to punch out the spectrum collected onto paper tape, to type the spectrum out on the typewriter, to spectrum strip, to zero the memory region associated with the analyzer, and to control the display of the spectrum on the oscilloscope.

With this system, it is possible to display either one or two of the four possible analyzer spectra on the oscilloscope at one time. It is also possible to overlay the display of the spectrum from one analyzer as compared to another analyzer. The use of markers (lower and upper markers) permits bracketing of a peak and subsequent expansion of this particular area of the spectrum for closer inspection. The markers, so called, are also used to control the typeout and punch-out so that only data between the upper and lower markers are typed or punched out.

Figure 3 shows the oscilloscope displaying a typical display where No. 1 is displayed on the left and No. 2 on the right. The analyzer being displayed is indicated by the number of dots present in the left-hand portion of the display. A typical single analyzer display is shown in Fig. 4. As is noted in both of these displays, the channels 32, 64, and so forth are indicated by means of a small mark at the bottom of the display. Figure 5 shows a typical single display where the markers have been moved in to bracket a peak of interest. Figure 6 shows this display as expanded. Figure 7 shows a typical display where two analyzer spectra are overlaid. This is done to compare the spectra collected presumably from like samples.

Figure 5 Bracketed spectrum peak in single analyzer display.



The "automatic" portion of the code is used to compute the isotopic content of a spectrum collected from an unknown sample. This portion of the code uses the mathematics described above to analyze up to eight isotopes by means of a weighted least-squares procedure. Previous to this analysis, it is necessary to collect background spectra and these are filed on to magnetic tape unit no. 4. In addition, it is necessary to collect standard or reference spectra.

Because of the extensive length of the "automatic" portion, a CHAIN-LINK procedure was introduced into this code which is similar to that used in a number of FORTRAN systems on other computers. The code was arranged in

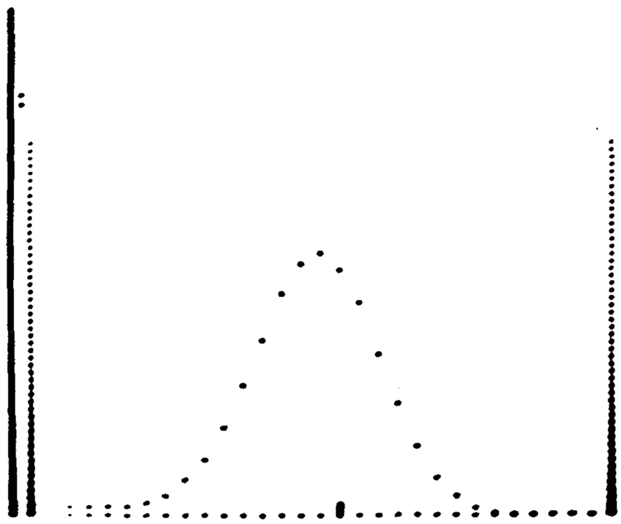


Figure 6 Expanded bracketed spectrum peak in single analyzer display.

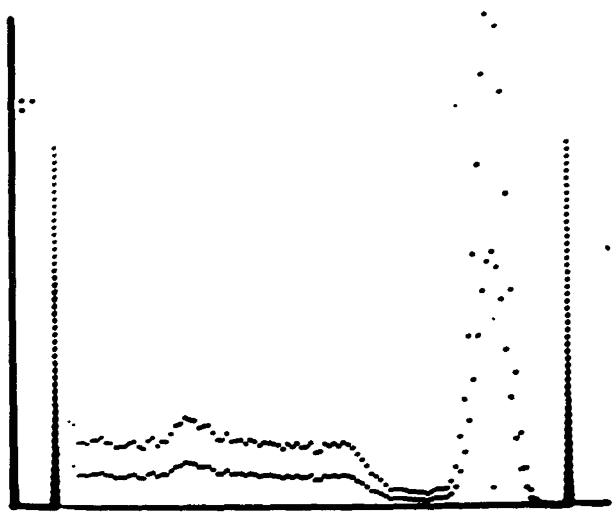


Figure 7 Typical overlaid dual analyzer display.

memory so that those portions which were necessary to service the interrupts, operate the display, and operate the magnetic tape units were all located in cells 0 to 1577 octal. The memory area from 1600 octal to 4177 was designated to be used for the CHAIN-LINK procedure. Thus, whenever a LINK portion of the code was brought in from magnetic tape for execution, it was brought in to this later area. Using this procedure, a code of approximately twice the size of the core memory of the computer was able to be operated.

Whenever any magnetic tape operations were in process, a program switch was set such that no further commands could be accepted by the Teletype input keyboard. This switch caused the portion of the code used to interrogate the keyboard to be bypassed and only the display portion of the code to operate. When any program required magnetic tape operations, this switch was set and the oscilloscope display would continue to be present, but it would not be possible to cause any program changes due to entries from the keyboard.

The code has been described in much more detail in two documents.[11,12]

System usage

The procedure followed during a typical sample analysis is as follows. Initially, after a cold startup general information is supplied to the computer memory using several different Teletype keyboard-driven routines, e.g., current time, sample reference time, isotopes present, miscellaneous instrument calibrations, analyzer live time, channel grouping. The computer memory is dumped onto magnetic tape for later retrieval so that the above typed input is not required every time analyses are performed and the computer is started up cold.

Background counts are then collected and filed on magnetic tape. Standard samples containing known concentrations of a single isotope (at the reference time) are then counted in all the geometries and for each analyzer upon which unknown like samples will be analyzed. The spectra are grouped, identified and filed by the computer onto the "standard's" magnetic tape.

At this point, analysis of the unknown samples which contain isotopic mixtures can be begun. The operator places the samples in the caves and starts the process for, say, analyzer no. 1 by typing an "A1." The computer then requests the sample identification, type of sample and the shelf that is being used. After the input information is complete, the computer signals return to command mode by typing a string of "*". After the counting live time plus two minutes (computation and tape searching time) has elapsed, the sample isotopic analysis is typed out along with the associated standard deviations and the normalized chi-squared. The computer then asks if the analysis is to be saved and the operator types Y or N accordingly. If Y (yes), the sample analysis is filed with its identification onto magnetic tape. Sometime later, these analyses are sorted by another computer code and the results reported in tabular form.[13]

Because of the real time aspects of the coding, the computations, tape searching, and typing out required during the analysis of a collected spectra from one of the four analyzers can proceed simultaneously with collection of spectra for any or all of the other analyzers.

Conclusions

The on-line system described in this paper has been operational for about 2.5 years. Over 12,000 samples have been analyzed in a rapid and systematic manner. Up to 125 samples per shift have been analyzed, the limit being determined by the live times used.

The expected benefits derived have been many: much lower cost of analysis per sample, immediate results, complete records of the sample analysis for verification in case of operator error, rapid availability of reduced data to the engineers in charge of the experiment, etc. In addition, one unexpected benefit has resulted. It has been found that if a long-lived standard is analyzed as an unknown and thus compared with its previously recorded value on tape, the chi-squared value is a most sensitive parameter for use in adjusting the gain and zero shift for the analog-to-digital converters.

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