

# Improved Productivity of a Radiotracer Detergency Method by Increased Automation

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## ABSTRACT

Productivity of a radiotracer detergency test method which generates several thousand samples per year has been substantially improved by automating record-keeping, data capture, data analysis storage and report generation. A group of programs has been written to acquire large amounts of data from liquid scintillation counters, a gamma counter and pH meters. The programs also maintain detailed records of each sample (swatch of fabric), provide current status of all swatches entered into the system, and make all calculations necessary to generate final test results. A Burcon microcomputer operating in a time-sharing mode allows multiple users to perform laboratory operations simultaneously. The programs (written in PL/I) are all interactive and the terminal screen displays provide a list of possible responses (menu) at each step. These menus, combined with careful design of the screen displays, minimize the amount of operator training necessary to complete processing successfully. The amount of operator time required to complete data processing has been reduced by ca. 35% and the automating of record-keeping and other tasks has further improved productivity and reduced turnaround time. A brief description of the component programs is included.

## INTRODUCTION

Since approximately 1966, Shell Development has used radiolabeled soils as a screening tool for detergency performance (1). The complexity and the use of this method has increased since that time so that the experimenter has a choice of several different oily soil types or combinations of types, with or without particulate soil, or particulate soil only (2-5). Briefly, the method involves soiling fabric with a clay (made radioactive by nuclear reactor irradiation), then adding an oily soil (such as an artificial sebum) labeled with hydrogen-3 (tritium) and/or carbon-14 and then washing the fabric. The predominant isotope in the clay is europium-152, which emits several penetrating gamma rays which can be counted directly with a NaI/photomultiplier scintillation detector. The soft beta particles emitted by tritium and carbon-14 are detected by adding wash water samples to an aromatic solvent/surfactant/fluorescent solution and counting the light pulses emitted. The application of this method to several detergency programs has previously been described (6-8, for instance). More than 5000 samples are run per year, requiring more than 20,000 analyses. To obtain final detergency results, four series of independent measurements must be brought together and correlated with the experimental parameters.

From the start, computer data processing has been used to convert the radioactivity counting data to percentage soil removal, and to produce a printed copy of the results (9). However, there was no provision for a project status record, nor was there an index to locate the partial results from a project. Further, the data reduction routines used were originally designed for punched card input to a local batch computer, but later modified to be used in a remote terminal, time-sharing environment in a central computing facility. Data entry into the central computer was one of the more time-consuming problems, so we decided to record data directly on the disk of a dedicated microcomputer which would then handle all the data reduction. Since all the programs were to be rewritten, we considered how we could better integrate the method to increase its productiv-

ity. It was obvious that one major need was better information management. Figure 1 shows a block diagram of the operations sequence. For any project, laboratory operations, counting and data reduction follow an interlocking sequence. The amount of clay on a soiled swatch must be determined by counting and the swatch is held in inventory until it is needed. When oily soil is added to the fabrics, the soil solution is assayed by counting. After the swatches are washed, the fabric and aliquots of the wash water are counted. All the counting results are then combined to calculate the detergency for each set of swatches. A project often requires several weeks from initiation to completion and several projects are usually in various states at any one time. This requires a large amount of data storage and, in turn, requires substantial programming to keep track of the data. Therefore, after the overall program requirements were outlined, a system was designed which would accommodate these requirements.

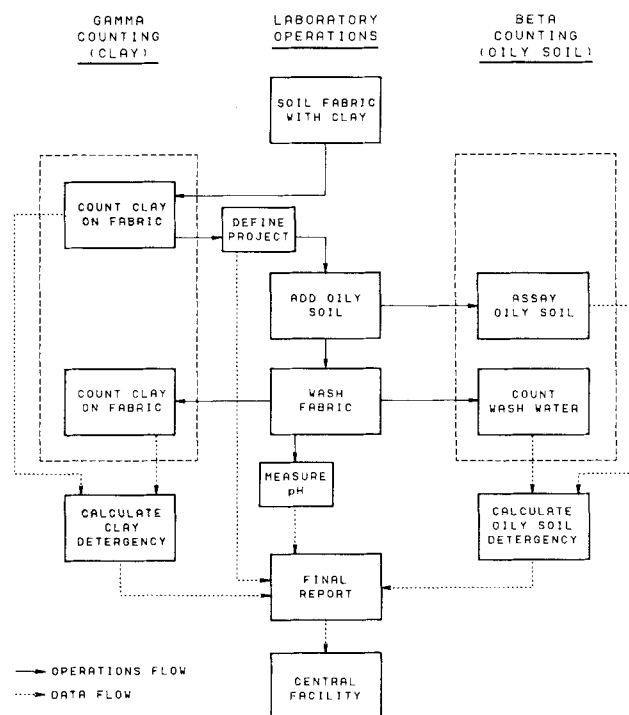


FIG. 1. Block diagram of radiotracer detergency method.

## SYSTEM REQUIREMENTS

### Data Inputs

Input data are generated by two liquid scintillation counters and a gamma counter which operate continuously and generate a reading every few minutes; by pH meters in the Terg-O-Tometer beakers, which generate five readings each during the 10-min wash (all of these instruments need to be interfaced to the computer), and input terminals for manual data entry. It is not practical, for instance, to halt manual data entry while the counters are operating, so

time-sharing capabilities are required.

**Data Storage**

Swatches are soiled with clay in advance of need. The inventory is generally about a thousand swatches or more, plus those in use for current programs and swatches from completed programs which have not been purged from the system. Counting data files are quite large and need to be retained until the related swatch data is purged. Thus, a hard disk system is needed.

**Data Presentation**

Manual data entry and prompting by the computer can be handled on a printing terminal such as a Teletype 43 or similar device. However, display rates are limited to the maximum printing speed, which is generally 30 or 120 characters per second. Video display terminals have a much faster display rate and can save substantial amounts of operator time. Additionally, carefully formatted screen displays aid the operator to interact with the computer. However, a printer is required for hard copy.

**Data Transfer**

After all detergency results have been obtained and verified, the data must be developed into a report, requiring statistical evaluation and graphical presentation. Since routines for these processes had already been developed to a high degree of sophistication in the central computing facility, the relatively small files containing the detergency results would be transferred to the central facility via telephone modem and the graphical presentations would be generated there.

**Computer System**

- Burcon System 85 microcomputer, based on the Intel 8085 CPU (Burcon, Inc., Houston, TX)
- CDC 96 megabyte capacity disk drive (Control Data Corporation)
- Televideo 950 CRT terminals for system console and data entry (TeleVideo, Inc., Sunnyvale, CA)
- TI 820 printer for hard copy output (Texas Instruments, Inc.)

The computer operates under MP/M® (© Digital Research, Inc.), version 1.0, the multiple user version of the CP/M® operating system. Substantial modifications were made to MP/M to reduce its memory space requirements without altering its characteristics (see Appendix). All programs were written in PL/I, since this language is very well suited to structured programming, manipulation of string variables, and indirect addressing (10).

Video display terminals allow rapid output to the screen for operator intervention. Each operation requiring operator action has a formatted screen to prompt the operator for the necessary responses. Figures 2 and 3 show typical screen formats. Such "friendly" programming minimizes the operator training needed to obtain the final results from the experiments, and minimizes the refresher training needed by occasional and back-up operators.

Transfer of the completed data file to the central facility is via telephone line at 120 characters/sec. A modem installed in the microcomputer dials the central facility, invokes the required protocol and transmits the data file with a single command by the operator.

Data from the pH meters located in the detergent applications laboratory (located ca. 500 ft from the counting laboratory where the computer is located) are transmitted by a custom-designed microprocessor interface device (see Appendix) over a line to the computer.

**Detergency Test/Computer Interaction**

The detergency test method and the data processing were developed over a period of years without a significant degree of integration, and as the method increased in complexity the volume of data transcribed and passed between the radiochemistry and detergent applications laboratories increased substantially. A major goal of this work was to automate passing data and to eliminate transcribing of data. The interaction of the detergency test method with the computer programs is described below.

Swatches soiled with clay are held in inventory. After a batch of swatches is soiled, each set is numbered and its level of clay-soiling determined by counting the gamma activity. This activity is recorded in a file automatically created for each new swatch by the program SWATCH. All subsequent operations and data involving a swatch will be

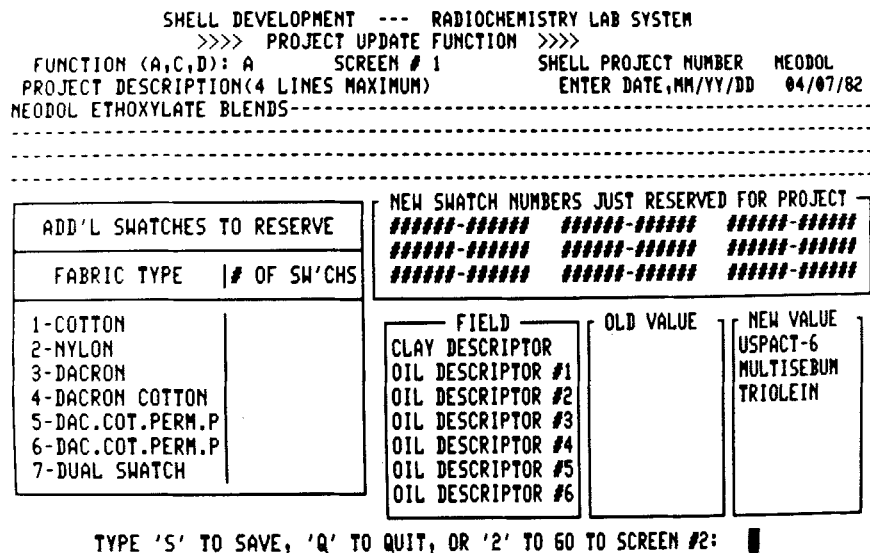


FIG. 2. Screen menu for initiating or updating a project.

## RADIOTRACER DETERGENCY METHOD

SHELL DEVELOPMENT ---- RADIOCHEMISTRY LAB SYSTEM  
 >>>> BETARUN CROSS-REFERENCE ROUTINE <<<<<

BETA MACHINE # : 1                      RUN NUMBER : 5

SAMP	SWATCH(ES)	SAMP	SWATCH(ES)	SAMP	SWATCH(ES)	SAMP	SWATCH(ES)
31	M2	130	X131				
31	600001-600010	131	M2				
51	600012-600050	131	600053-600067				
129	M1	161	S				
129	600051	161	█				
VERIFY & SAVE S							

MODE CODES	NO SWATCH 600067
SINGLES/DUPES/TRIPLETS	
M1 █ M3	
POSTWASH/RE-DEPOSITION	
█ M7	

#####	- 6-DIGIT NUMBER
#####-#####	- RANGE OF 6-DIGIT NUMBERS
X###	- SKIP TO SAMPLE POSITION ###
M#	- SWITCH TO MODE # (SEE LEFT)
(BLANK LINE)	- SKIP TO NEXT SAMPLE NUMBER
Q	- QUIT ... DO NOT SAVE
S	- SAVE, PRINT A REPORT & QUIT

FIG. 3. Screen menu for cross-referencing a liquid scintillation counting run, showing input from operator.

recorded directly or indirectly in its swatch file.

When a detergency test project is designed, the chemist in the detergents laboratory calls up the PROJECT program and enters the project parameters, including detergent formulations, fabrics and soil types, according to the prompts on the display screen. The program records the project name, and checks the inventory of soiled swatches and looks for the smallest, sufficient group of swatches from the same clay-soiling batch. The program then reserves these swatches by entering the project number in the file of each swatch.

When the oily soils have been applied, the user enters OILYSOIL, types the project number and the swatch numbers for each oily soil.

The program PREWASH generates a Terg-O-Tometer run sheet for use at wash time.

At the time the swatches are washed, the program WASH queries the interface device which reads the 4 pH meters, formats the data and returns the data to WASH. WASH then records wash liquor pH values at five times preselected by the user. The program displays the data entered previously from PREWASH, and the user can make any changes desired. The user then indicates that the wash is starting and the system monitors the 10-min wash by pH.

After the wash is completed the fabric is removed from the beaker and rinsed by hand in clear water. Aliquots of the combined wash and rinse water are added to liquid scintillation solution to measure tritium and carbon-14 activity to determine oily soil removal. The wet swatches are placed in a plastic vial for gamma counting to determine the clay removal.

The samples are taken to the radiochemistry counting laboratory and placed in the appropriate counters, along with background and calibration standards. The programs BETARUN and GAMMARUN initiate recording of the counting data. BETAXREF, GAMAXREF and ASAYXREF correlate counter run number and counter sample position number with swatch or assay number. The sample position and swatch number are entered manually (see Fig. 3) and the program then updates the swatch files, as described above. These cross-reference programs constitute the bulk of the manual data entry required.

After the counting has been completed and the cross-reference has been made, the data reduction is carried out by BETALYZE and GAMALYZE. These programs calcu-

late calibration functions and perform statistical analyses of the data. Each provides a printout of the calibration and counting data to allow monitoring of counter operation, counter stability and sample stability. Counting variations which exceed preselected limits are flagged to aid the operator in the identification of questionable data and/or results. Figure 4 shows an example of the results from BETALYZE.

ANALYZE takes all the data from a project, calculates detergency results for all soil components and prints a report containing all the variables, initial and final pH readings and detergency results for all beakers, along with the average results for replicate washings. These results are also stored in a file which the program CMSLINK sends to the central computing facility for use by the detergent applications laboratory. Figure 5 shows an example of the final output from ANALYZE.

All the programs allow for correcting or adding to keyboard input at some later time. Malfunctions of the counters sometimes cause a sample to be skipped in the sequence, or a sample may be obviously invalid. Rather than recount a complete sample string, which may take two or three days, EDIT allows the operator to inspect any counting data before or after data reduction, make any required adjustments and then reprocess the data. Only the latest version of the results is saved in the computer.

The logic flow of the programs is shown in Figures 6 and 7. The structures of all the data files are shown in the Appendix.

## RESULTS AND DISCUSSION

The system described above has been in use for only a short time, but our experience to date shows substantial cost savings due to (a) ease of operator training, (b) increased reliability of data input to the microcomputer compared to the central facility, (c) direct recording of experimental parameters and other data, and (d) automated project status records. From project inception to transfer of the final data, identification of swatch number with the position number within the counter is the only hand-written record required. Increased use of statistical analysis of counting data with automatic flagging of questionable values for the operator's attention has increased the data reliability while reducing the operator time required for



## RADIOTRACER DETERGENCY METHOD

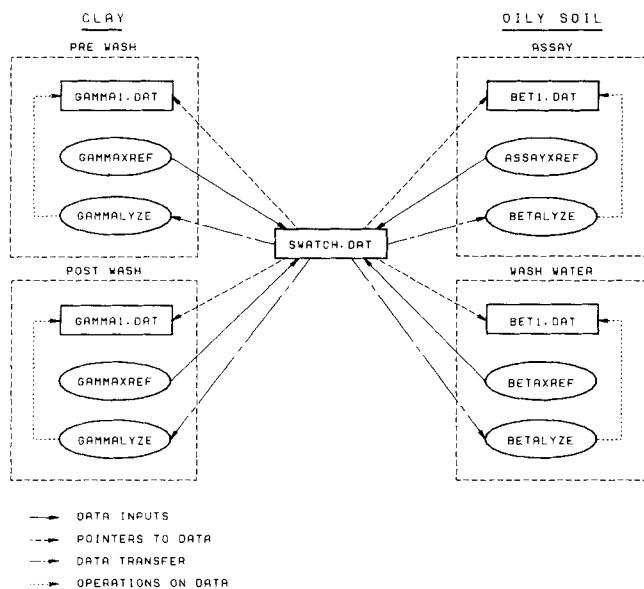


FIG. 6. Logic flow in labeled soil calculations.

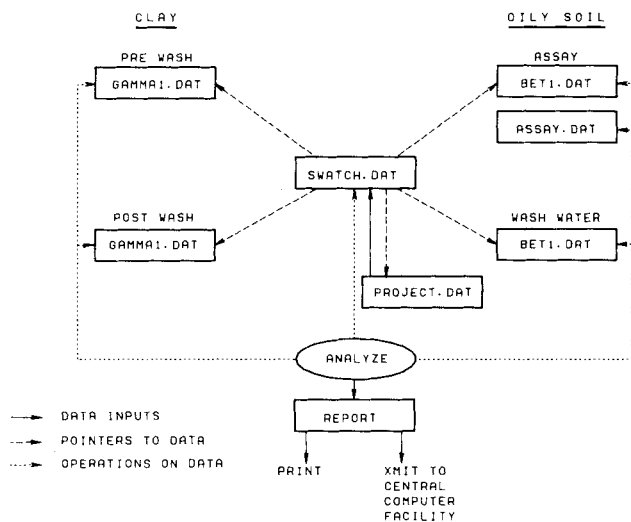


FIG. 7. Logic flow in detergency calculations.

data evaluation. These flags catch most sample and counter errors. However, not all errors are caught in this manner, nor are their causes always obvious. Therefore, the decision to use or reject any data is up to the operator. Based on the current level of operations we project an overall labor saving of 0.5 man-years per year due to this system.

Several enhancements to the system are under consideration for the future. A new version of the MP/M operating system, MP/M II® (© Digital Research, Inc.) is available. The new version contains several desirable features (password capabilities which could prevent inadvertent loss of files, more flexible operations, etc.) and will be added to the system when others have accumulated sufficient experience with the new version. CP/NET®, a control system for networking microcomputers in the MP/M environment, is also under consideration. Under CP/NET, a small microcomputer with 64 kbytes of memory and dual 8-in. disk drive could access data files on the large disk, run the data reduction routines and write the results to the large disk for transmission to the central facility. Such an arrangement would allow the large system to be used mainly for data

acquisition and may become necessary as additional remote detergency stations are added to the system.

## ACKNOWLEDGMENT

J. A. Vento wrote the data editing and file purging programs. R. T. Pennington interfaced the instruments to the computer. W. M. Savage of Burcon, Inc., wrote the BETALYZE, GAMALYZE and ANALYZE programs, plus many system routines.

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## APPENDIX

## MP/M Modifications

The MP/M operating system is designed to handle from 1 to 16 consoles. A console need not, however, be a terminal. The Terg-O-Tometer and the three counters were to be referenced as 'console' devices. The original design was for 3 terminals, 3 counters, a Terg-O-Tometer, plus any additional consoles for expansion. Using MP/M, each console added after the first two requires 256 bytes of memory. The large number of devices produced an operating system that dwarfed the amount of memory available for program development. Therefore, the MP/M operating system was modified to include three consoles.

The Terg-O-Tometer and three counters now have their own system queues. These queues are an MP/M facility requiring a minimal overhead of ca. 24 bytes per queue + length of the queue in bytes (1 character = 1 byte). An assembly language program is continuously running behind the scenes, sampling each machine for data every clock tick (50 ticks = 1 sec).

## Computer/pH Meter Interface Design

A custom interface was required between a Burcon computer and four DataTech, Model 14 (DIGIPHASE) pH meters. The pH readings calculated by DataTechs are available on the back of the units. The output consists of 3½, binary coded decimal (BCD) digits and three status lines driven at standard TTL levels. Upon command from the Burcon, the interface must scan the pH meter's BCD output, determine if the data are valid, convert the readings to an ASCII string, and send the information out on an RS-232 compatible serial port to the computer.

The interface is a microprocessor based system, designed using 'STD bus' printed circuit cards. Board level design was chosen because of the ease of implementation and maintenance. The STD philosophy calls for a variety of cards, each performing a unique function, that plug into a single card rack. To configure a system the engineer selects the cards he needs to perform the required functions, inserts them into a card rack, and programs the local processor. If the

system fails, the problem card can be isolated because of its unique function and replaced.

The interface must be able to read the TTL signals from four meters, manipulate the data obtained from these signals, and send information out on an RS-232 serial port. To perform these tasks the following ProLog, STD bus, printed circuit cards were required:

- A Z80 microprocessor card (ProLog #7803) with on board random access memory (RAM) and read-only memory (ROM) to control the interface.
- A dual universal asynchronous receiver transmitter (UART) card (ProLog #7304) which allows the interface to communicate with an RS-232 compatible device.
- An input card (ProLog #7603) with 64 TTL compatible inputs to read the outputs of the pH meters.
- A power supply card (ProLog #3000) which is used to generate +5, +12 and -12 volts.

The boards are connected by the STD bus card rack. The rack was mounted in a suitable metal box. A power switch, power indicator and a reset button were added. RS-232 signals were brought out to a standard, 25 pin, female, D-type connector. The BCD signals were wired to individual, 37 pin, D-type connectors.

### Operation

When the computer requires the current pH readings it must prompt the I/O box for the values. The computer must send an ASCII character number 5 (ASCII-5), the enquiry character, to signal the interface to send data. All other characters will be ignored by the box. After the prompt is received, the interface will read the pH meters and send the computer the four values. All readings will be sent as four digit numbers, transmitted as an ASCII string with an implied decimal point after the first two digits. Values will be separated by an ASCII-9, the tab character. The string will be terminated with an ASCII-13, a return, and an ASCII-10, a line feed.

If the interface detects a bad number from the pH meter, it will re-try the reading up to 5 times. Should the I/O box not be able to obtain a good reading, four nines will be sent to the computer in place of the uncertain number.

The interface will ignore all commands from the computer while the pH values are being read or processed.

A typical basic language computer would use the following statement to prompt the I/O box for the current pH values:

```
PRINT CHR$(5)
```

Execution of this command will cause an ASCII-5 with no line-terminating characters to be sent to the interface. Immediately following the print command the computer should execute:

```
INPUT PH1, PH2, PH3, PH4
```

This command will allow the computer to receive the four new values.

### File Structures

*Swatch.DAT.* This file contains all information describing a single swatch. One record contains: (a) project number;

(b) swatch number; (c) clay descriptor; (d) oily soil, assay and detergent numbers; (e) 12 user-defined variables; (f) pointers to the raw counting data in the Beta and Gamma files; and (g) 5 pH values taken from the Terg-O-Tometer.

*Project.DAT.* This is the project file. The one record in this file contains: (a) clay descriptor; (b) 6 possible oily soil descriptors; (c) 6 possible detergent descriptors; (d) all label fields for the 12 user-defined variables; and (e) the project name.

*Bet1.DAT.* This file contains all information concerning Beta machine #1, a Packard Model 3385 liquid scintillation counter. A single beta run consists of 17 physical records. Beta record-1 contains the header information, including: (a) time/date of collection; (b) status (not working, working, done) of the run; (c) status of the cross-reference; (d) status of the analysis; (e) the pass count; (f) position of the last sample in the counter; (g) the normalized polynomial calibration functions for the tritium and carbon-14 standards; (h) the position of the first standard sample; (i) the activity of the standards in disintegrations per minute; and (j) the analyzed data for the first 100 positions.

Beta record-2 contains analyzed data for up to 200 sample positions.

Beta record-3 contains the raw counting data in a 20 sample by 5 counting cycle structure. There are 15 Beta record-3s in this file.

*Bet2.DAT.* This file contains all the information concerning Beta Machine #2, a Packard Model 460C liquid scintillation counter. A single BETA run for this counter consists of one Beta record-1, two Beta record-2s, and 23 Beta record-3s. All other information is the same as for Bet1.

*Gamma1.DAT.* This file contains all information concerning a GAMMA run from a Packard Model 5220 AutoGamma counter. A single GAMMA run consists of one Gamma record-1, one Gamma record-2 and 12 Gamma record-3s.

Gamma record-1 contains: (a) time/date of collection; (b) status (not working, working, done) of run; (c) status of cross-reference; (d) status of the analysis; (e) the pass count; (f) the last position in the sample string; (g) the expected count rate of the Cesium-137 standard; and (h) the analyzed data from the first 150 sample positions.

Gamma record-2 consists of analyzed data for up to 156 positions.

Gamma record-3 contains the raw counting data in a 25 sample by 5 counting cycle structure.

*Assay.DAT.* This file contains all vital oily soil assay information related to one particular assay run. One record represents a complete ASSAY run including: (a) All specific activity data (in disintegrations per minute per milligram of soil) for the 15 assays; (b) Beta machine number; (c) Tritium specific activity; and (d) Carbon-14 specific activity.

*Wash.DAT.* This file is used to store temporarily the information for a particular project's wash run sheet. Space is available for up to 20 projects. When washing is completed and the reports are complete, the run sheet for a project can be deleted.