

# A Review and Experimental Evaluation of Commercial Radiocarbon Dating Software

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### ABSTRACT

New commercial radiocarbon dating computer software has been developed to provide on-line data analysis for Packard computer assisted counting systems and off-line data analysis for other instruments. Because different radiocarbon laboratories may have slightly different methods of calibration and data presentation, the software was designed based on the routine methods and calculations performed at the Center for Applied Isotope Studies (CAIS). Input from several other radiocarbon laboratories was also incorporated in the design of the computer software. This chapter presents a complete product critique, from a users' point of view, covering ease of use, calculations, and future applications of radiocarbon application software. Comparative data will be presented to show the differences between this radiocarbon software data analysis and the routine data analysis that is performed at the Center for Applied Isotope Studies.

The software is menu driven with on-screen programming and editing for a professional user interface environment. It also has the capability to save and analyze counting data directly from the Packard liquid scintillation system. The software can be programmed to accept oxalic calibration information and count data. The software data disk management develops count history files of a carbon reference standard and background over time. The user can archive data into a unique data subdirectory. Data can be selected to export collected and stored information for incorporation into other computer software such as Lotus<sup>R</sup>1,2,3<sup>R</sup> or database programs.

The software offers several correction features, including an account of benzene evaporation and Delta <sup>13</sup>C isotope value, and it can be programmed for the scintillation counter radionuclide efficiency.

### INTRODUCTION

Laboratories that specialize in low level radiocarbon measurements as a part of their own research programs or as a commercial service to the scientific community have had to develop in-house computer software to automate these routine calculations. A question often raised by new laboratories that for the first time enter into low level radiocarbon measurements concerns the analysis and interpretation of the counting data. In many cases this question remains

unanswered until a literature search through the annals of *RADIOCARBON* uncovers the commonly used calculations and methods of correction for radiocarbon age dating. It is not uncommon to discover a startup radiocarbon laboratory that has limited knowledge of these calculations and how to apply the correction schemes.

The application of laboratory computers used in routine data analysis for a specialized task like radiocarbon age dating has, in the past, required a programmer/scientist to develop and test the software used by the laboratory. In the absence of computer software, hand calculations would suffice.

When we learned that specialized application commercial software was being developed for radiocarbon age dating analysis, we became interested in evaluating and comparing the results of the new software package to our own radiocarbon analysis program.

## **BACKGROUND**

The radiocarbon software was developed by Packard Instrument Company of Downers Grove, IL, for use with the computer assisted, as well as the noncomputer automated, line of liquid scintillation counters that the company manufactures. At the time of this independent product evaluation, the software has not been released for commercial distribution. The software provided for our studies was a prerelease version. The software as we know it was intended for on-line data analysis using the Packard Tri-Carb® series models 2260, 2250, 2200, 1050, 1000 liquid scintillation analyzers. Off-line data entry and subsequent analysis does not seem at this time to be an option of this software. The liquid scintillation analyzer used in our evaluation was a Packard Tri-Carb model 2050, predecessor of the model 2250, both are specially designed low background counting systems.

## **EVALUATION CRITERIA**

This product evaluation was conducted solely on the basis of an individual end user. The software was evaluated in five areas of interest; (1) installation and documentation, (2) ease of use, (3) correctness of calculations, (4) user benefit features, and (5) future applications.

In order to compare results obtained from the new Packard software to the data analysis performed at CAIS, several wood samples from the radiocarbon laboratory at the University of Waikato in New Zealand were dated using both computer programs. The samples of wood ranged in age between 2,000 years before present (YBP) to approximately 50,000 YBP. All sample dates were corrected for carbon isotope fractionation. The opinions expressed here are those of the authors and do not represent those of Packard or the University of Georgia.

## MATERIALS AND METHODS

Each wood sample was prepared for liquid scintillation counting by first cutting away the surface related wood material and then successively pretreating it with chemicals to remove possible contamination from modern carbon components. The treated wood sample was processed to pure benzene using a benzene synthesizer. A 3 cc sample of benzene was derived from wood combustion and mixed with scintillators; counting followed.

The samples were first counted using the CAIS scintillation counters, normally used to process routine samples. Each sample was counted for 2700 minutes in a Picker/Nuclear Liquimat 220 with a specially designed low background copper/Teflon®\* shielded counting vial, and then the age date was calculated.

Originally, the counting experiment was designed for the CAIS system and the Packard software to be similar. It was later discovered that the Packard software was designed to count each sample once, unload, and cycle it around the sample changer before counting for a repeat time. To minimize statistical variations due to cycling, each sample was counted for a single 999 min interval, and then the date was computed using the Packard software. Normally at CAIS, each sample, background, and oxalic standard is counted in the same counting vial because each liquid scintillation counter is calibrated with its own vial to minimize experimental variations. Using the Packard system, the software is designed to count the sample in a multi-user environment. This means that the investigator should place the samples in a cassette in a desired sequence. This sequence can be programmed by the user into the software, so the software can recognize the difference between a standard, background, oxalic, and sample. However, this multi-user environment does not lend itself to counting each radiocarbon sample, oxalic, or background in the same counting vial. To accomplish this, the investigator must manually intervene to stop the counting system, prepare a new sample in the same vial, and start the counting again. This system works best when using a different vial for each sample. The counting vial used with the Packard counting system was a standard low <sup>40</sup>K borosilicate glass vial with an internal volume of 7 cc. Teflon cap liners were used to prevent solvent loss during the counting interval.

## HARDWARE AND SOFTWARE REQUIREMENTS

The software was developed in the "C" programming environment and runs on an IBM Personal Computer (PC) or Professional Series (PS) micro-computer system and compatible. The computer in any case must be compatible with the interfacing to the Packard scintillation counter and the executing of the scintillation software. The radiocarbon application software is an add-on program that runs within the scintillation software operating environment

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\*Teflon is a Registered Trademark of E.I. DuPont de Nemours

on computer assisted counting systems. Using the Packard Datalink™ stand alone counting systems like the Tri-Carb model 1050 the investigator can compute age dates with the radiocarbon software. No additional computer equipment, other than what is typically provided with each Packard counting system, is required for operation. During the software installation, the color option can be activated for use with top of the line Packard counting systems, which are equipped with a color monitor.

### **Installation and Documentation**

Since the software provided for evaluation was a prerelease version, the documentation supplied was not the information that would accompany the commercially released product. At this time, we cannot describe the quality or completeness of this material.

The program installation was complete. The original disk, provided in the 5.25 in. floppy format, contained an installation routine that prompted the user for the different Packard counting system models. Since the Packard system used was an earlier vintage, the use of subdirectories was not supported. The radiocarbon software was then installed to the root directory on the hard disk, which contained all other files used to operate and communicate with the scintillation counter. Newer models of Packard counters support the use of subdirectories, making the house keeping of different files of a given software package much easier.

### **Ease of Use**

Once installed, the software was very easy to access through the Packard scintillation software user interface. The radiocarbon program was developed as a menu driven system with preprogrammed function keys for different operations and modules. The Packard operating environment allows application software, like the radiocarbon program to execute and run while the scintillation counter was performing the most recent instruction from the scintillation software. If the scintillation system was counting a sample when the user executed the radiocarbon software, the sample would continue to count until its time or statistical termination was satisfied. At that point, if the scintillation program was not returned to the main portion of memory, the counting system would wait until the user terminated conversation with the application program before the counter would go on to the next instructed task. A safety feature of the system is that it can sense keyboard activity. If the user executes the application program and is called away from the computer, the program will automatically terminate, saving the most recent information and returning to the operation of the scintillation counter within a preset period of time.

The use of eight preprogrammed function keys enables the user to navigate through the system as shown in the flow chart (Figure 1). There is a help line at

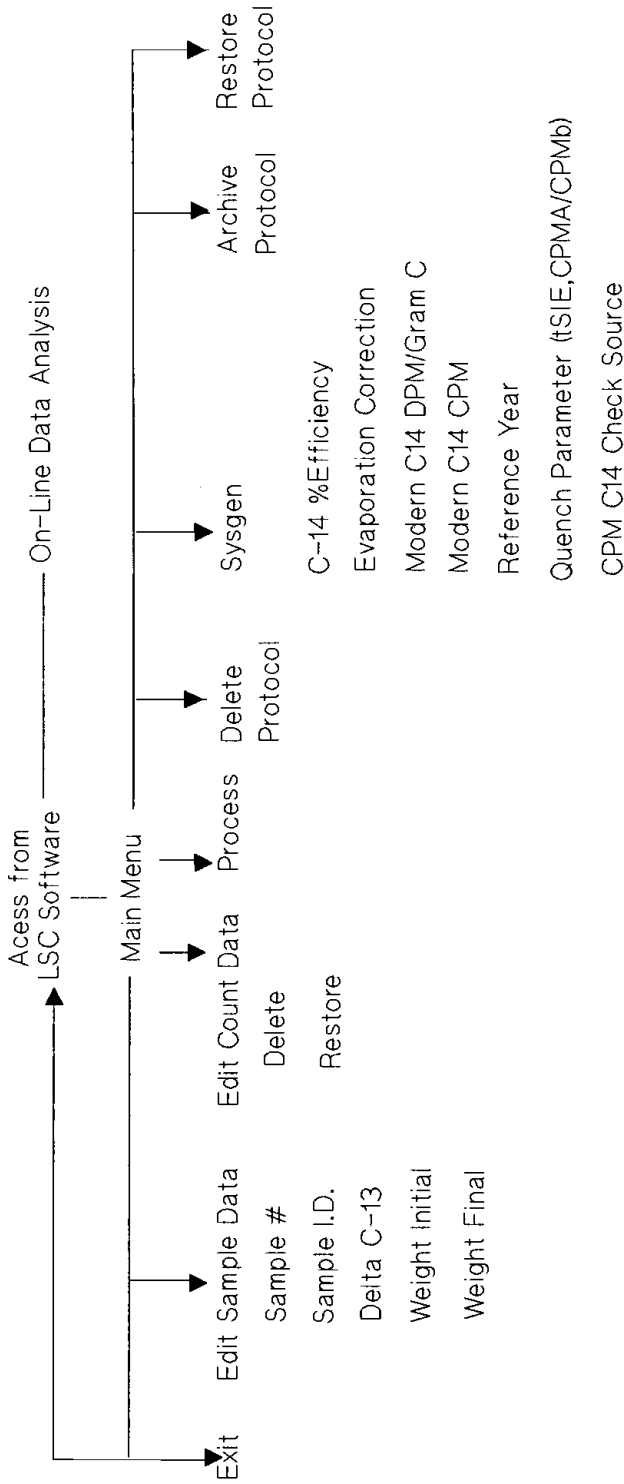


Figure 1. Radiocarbon software flow chart.

the bottom of each screen to provide expected responses for software prompts.

Once the counting protocol in the radiocarbon software has been predefined by the user, all that is required is counting the sample. The subsequent data analysis is automatic, a printed report follows. The protocol defined in the radiocarbon software must be identical to the counting protocol on the scintillation counter. The radiocarbon software can be user programmed through the scintillation software to process the sample data after each sample is counted (Sample Mode) or after a contiguous group of samples is counted (Batch Mode). However, in Batch Mode, the radiocarbon data analysis and report are not generated until the logical end of the group. So, if each sample is programmed to count for 1000 minutes, it could be some time before the radiocarbon age of the first sample is reported.

Overall, the software can automatically calibrate, based on the user providing the correct oxalic reference information, weight of the sample in terms of benzene, and Delta  $^{13}\text{C}$  data. The user can edit previously counted data on-screen, should there be a need to delete or restore data. In addition, the user can achieve logical groups of raw sample count data and also export that information to a selected disk drive as an ASCII file for later import into other software packages.

## SOFTWARE FEATURES

### System Generation

One of the initialization functions the software provides the user is the ability to enter the externally computed  $^{14}\text{C}$  counting efficiency, oxalic acid specific activity, and the count rate of a check source. Other information regarding the correction of benzene evaporation is activated within Sysgen. The Sysgen screen allows the user to select or enter their own specific activity for the oxalic acid standard. Presets were available for oxalic acid I (SRM 49) of 14.27 DPM/gr C and oxalic acid II (SRM 4990-C) of 18.46 DPM/gr C. The software was designed to automatically compute updated counting efficiency information, check source CPM, and oxalic acid CPM when these samples were identified by the user and counted.

This screen appears to be simple in design, but the prompts were somewhat vague and should be explained in the final documentation. The software does, however, allow the user to enter a nondefined specific activity for the oxalic acid in the event that the user is not calibrating on oxalic acid, but possibly some other reference material.

### Edit Sample Data

The radiocarbon software provides lets user program each sample identification with a sample number corresponding to the position of the sample in

the cassette, the Delta  $^{13}\text{C}$  value, and the weight of sample benzene. When the evaporation question is activated through the Sysgen menu, another column of data appears on this screen, allowing the user to enter the final sample benzene weight. In order to correct the previous data for the loss of benzene during counting, the original count data must be manually reprocessed. The sample specific activity is corrected for the sample benzene loss by taking half of the difference between initial and final benzene weights. As a result of benzene loss, the percent difference between the initial and final weights are computed.

Once the sample data have been entered, the user can initiate counting and wait for the final results. This module of the software allows the user to program on what given date the calculation should begin.

### **Edit Count Data**

Once the samples have been counted, a count history file is generated for each sample. When a particular sample is counted repeatedly, the total counts for each cycle are combined and a correlation value computed. If the sample has counted for more than 5 cycles, an additional correlation value over the most recent 5 cycles is computed. This provides the user with information regarding the reproducibility of the count results. If there is any bias in the data, the counts/day are computed and printed.

In this module the user can selectively delete one or more count repeats. The program flags the deleted point(s), but does not discard the information. If the user wishes to restore the deleted point(s), the Restore function can remove the delete flag so that the sample data can be incorporated into the final calculations.

## **COMPARATIVE RESULTS**

In order to compare the radiocarbon age calculations between the CAIS routine method and the new Packard software, six different wood samples were processed to benzene and counted. These samples ranged in ages between approximately 2,000 YBP and 50,000 YBP. Also a modern oxalic standard was measured to see how the software would handle the 136% of modern sample. The benzene samples were measured in the standard CAIS counting vial when the sample was counted using the CAIS LSC spectrometers. The Packard software was designed to count each sample once and then cycle the sample, enabling the instrument to count another sample before repeating a given measurement. Because of this limitation, the same counting vial could not be used for the standard, sample, and background as was accomplished in the CAIS routine. Each benzene sample was transferred from the CAIS counting vial into a common 7 cc low  $^{40}\text{K}$  glass vial.

The comparative results are presented in Table 1. It was apparent that on the

**Table 1. Radiocarbon Age Dates—Charcoal Samples  
CAIS vs Packard Software**

| Sample I.D.<br>UGA | $\delta^{13}\text{C}$ | CAIS<br>YBP $\pm 1\sigma$ | PACKARD<br>YBP $\pm 1\sigma$ | % DIFFERENCE |
|--------------------|-----------------------|---------------------------|------------------------------|--------------|
| 5894               | -25.81                | 1,974 $\pm$ 50            | 2,019 $\pm$ 50               | 2.3          |
| 5897               | -25.85                | 2,036 $\pm$ 52            | 1,894 $\pm$ 50               | -7.0         |
| 5891               | -24.96                | 3,232 $\pm$ 419           | 2,894 $\pm$ 50               | -10.5        |
| 5903               | -24.67                | 5,058 $\pm$ 65            | 4,695 $\pm$ 50               | -7.2         |
| 5900               | -24.83                | 49,033 $\pm$ 7569         | 38,635 $\pm$ 50              | -21.2        |
| 5888               | -25.56                | > 50,000                  | -6E38                        | -            |
| Oxalic-4990C       | -17.68                | Modern                    | -2393 $\pm$ 50 (Modern)      | -            |

basis of counting these radiocarbon samples there were differences between the CAIS method and the Packard software. Most of the age dates computed automatically with the Packard software demonstrated a negative bias ranging from approximately 2 to 21% from the CAIS corresponding values. The software was executed, with no correction schemes activated, to yield computed age dates that were not influenced by any possible errors in the code.

Upon discussing the results, Packard is still in a program developmental stage. CAIS endeavors to assist the program developers at Packard in identifying the program errors so this commercial software package will carry the full merit of radiocarbon age dating capability.

## GENERAL COMMENTS

At present, the Packard software is in need of further debugging and testing before it is ready for commercial distribution. We believe that new startup radiocarbon laboratories will probably benefit the most from this on-line software analysis. Established laboratories such as CAIS and others around the world, most likely will continue to utilize their own developed radiocarbon software for computation of age dates. Since this software is closely related to the equipment of one particular manufacturer, it does provide the capability for new laboratories to obtain the counting equipment and analysis software from a single source and it is ready to use.

During our test and evaluation period, we had discovered several bugs in the program, some which prevented us from continuing with our evaluation. Packard responded quickly with programmer support to correct the apparent problems and provided us with another version. The program source code was not made available to us for modification, but we were pleased with the prompt attention from Packard.

## FUTURE APPLICATIONS

During the recent year, other radiocarbon laboratories have developed radiocarbon age date and radiocarbon correction type application software.

The Centrum Voor Isotopen Onderzoek in Groningen, the Netherlands, under Professor Van de Plicht, has made available to the radiocarbon community computer software that will provide tree ring corrections to radiocarbon dates. This software was developed in the Pascal language. Recently, a computer program named "CALI" was published by the Laboratorio de Datacion por Carbono-14 at the University of Granada in Spain. This program was developed similarly, to provide a calibration of radiocarbon age dates.

Although at CAIS, we have not had an opportunity to fully evaluate and compare these newest radiocarbon software packages, there appears to be a growing interest among different laboratories in the development of computer software for this specific purpose.

We believe that the direction many radiocarbon laboratories are considering is one that will completely automate the radiocarbon sample calibration process. Ultimately, once the sample is loaded into the counter, the computer software that controls the scintillation counter or acquires the data from a stand alone counting system will capture the counting data from the equipment, compute the radiocarbon age of the sample, and provide the different types of correction schemes. At present, the Packard computer-assisted counting systems can execute user-programmed software to further analyze the counting data. The on-line radiocarbon software, once fully operational, will provide radiocarbon calibration of samples counted, but it does not completely include all of the different correction schemes. The next logical step in the sequence of software development will be the linking of on-line radiocarbon software to the other programs developed to correct the calibration dates for a complete data presentation.

