

Chapter 21

Acquisition and Handling of Liquid Scintillation Counting Data

J. L. Spratt

*Department of Pharmacology, College of Medicine,
University of Iowa, Iowa, U.S.A.*

INTRODUCTION

Since all previous speakers have necessarily been discussing data handling and since all of the speakers following are specifically committed to the subject, I find myself in an unusual situation. Likewise, in contrast to the lecturers in other sessions, I am not a developer of liquid scintillation spectrometers nor do I devote a substantial part of my effort to investigating the basic chemistry and physics of the liquid scintillation process. I am a user of liquid scintillation counters and my view is from that perspective.

Not being a statistician, I chose not to dwell extensively on that subject. A detailed account of computer programming *per se* seemed inappropriate. I therefore chose to present a compilation of user considerations that could be applicable to old or new spectrometers, to old and new users, and could serve the reading audience as well as those present here. As the last plenary lecturer, it also appeared to be incumbent upon me to include a variety of loose ends which have been of concern to many as evidenced by both formal and informal discussion at this symposium.

Hicks has recently stated my general concern regarding the handling of liquid scintillation counting data when he discussed *The Computer: Is it the Solution or the Problem?* He said:

'Computer specifications generally emphasize the bits of precision in the floating point software, the speed of floating point hardware, the cycle time of the central processing unit, the speed and size of mass storage, etc. I submit that the discussions of such specifications are meaningless until it is known what type of problem is to be solved. The selection of an approach using small computers, a larger computer, or a mixture of the two can only be made once one has defined the problem and has some understanding of the proposed solution.'¹

Since it is my contention that excellent data handling is often performed on inappropriate data, I have chosen to incorporate data acquisition problems and pitfalls in this discussion. The presentation will be of an historical nature since the problems of data handling are necessarily commensurate with available hardware and software. Since the problems that face the specific user are uniquely his own, I will not provide you and readers of the symposium text with specific answers to your individual problems, but hopefully will provide some considerations and approaches which you may want to apply

to your own environment. Although such a survey will not allow for extensive discussion of many points, the bibliography will direct readers to many particulars.

After brief comments on a few review articles, the subject of performance parameters and instrumentation available will take our attention in a somewhat chronological fashion. We will then discuss types of quenching effects and approaches to quench correction. This will be followed by a discussion of statistical considerations and computer programs for data handling.

We will conclude with a discussion of factors influencing the data obtained in liquid scintillation spectrometry and will pose the considerations to be entertained when deciding whether to proceed with computational gear supplied with the spectrometer or to proceed with a variety of non-spectrometer computational approaches.

It is of interest to note that the 1969 Liquid Scintillation Conference in Boston² had sessions on data handling and the 1970 Conference in San Francisco³ had sessions on computer programming. On the other hand, the 1957 Northwestern Conference in Chicago⁴ had no such sessions since liquid scintillation counting was very much a manual procedure at that time. The various developments which have occurred since those early days have had great influences on the handling of counting data. The aforementioned symposium volumes, the book by Birks,⁵ Rapkin's earlier reviews,^{6,7} and his series in the Picker Nuclear Laboratory Scintillator in 1966-67, are all very useful references describing these developments.

Table 1. Developments influencing data handling.^a

Single sample	→ Multiple samples
Visual readout	→ Printed readout
Single channel	→ Multiple channels (channels ratio)
Gross count rates	→ Background subtraction and low count reject
Lister	→ Calculator
Printed readout	→ Punched readout
Internal standardization	→ External standardization
Calculator	→ Computer

^a Plus innumerable electronic and mechanical improvements.

INSTRUMENTATION AND PERFORMANCE PARAMETERS

Both liquid scintillation spectrometry and effective computers were born in the 1950's. By 1962 we had advanced to tritium efficiencies of 7% with a background of 52 c.p.m.⁸ Some of the developments which brought us to our current abilities are shown in Table 1. Multiple sampling and printed readouts meant that we could continuously monitor samples without personally attending the counter at all times. This meant we could now spend that time generating more samples and more data to overwhelm one another in the literature. Multiple channel machines allowed for less dial-twisting for some and more dial-twisting by others. The former took advantage of the development, the latter produced developments i.e. discriminator ratio techniques and the later channels ratio approaches to quench correction. Background subtraction and low count reject features had varying effects on data handling procedures. When solenoid decks were put on printing calculators, data reduction was much more convenient and tempted investi-

gators to do even more dial-twisting with resultant advances in quench correction techniques. With readouts being punched on cards or paper tape came the pivotal question of handling data off-line versus having the data handled on-line by the accompanying calculator or its successor, the built-in dedicated computer. The use of both external standardization and channels ratio techniques now vastly overshadow the old original internal standardization technique for quench correction.

Along with these developments came a greater degree of dependence on an extremely complex piece of apparatus that supplied us with very precise data – whether it was right or wrong. In this regard, it is appropriate to quote from Wyld's presentation⁹ at the Boston symposium:

'There was a time in the history of liquid scintillation counting when we knew very well we could have no confidence in the results from our equipment unless we counted everything ten times or more, and unless an investigator was something of a physicist and electronics expert, he was probably not even working in this field. Today, however, the situation is changed. We pay our money and in due course receive an instrument that is really a wonder to behold. Just looking at the awe-inspiring sight generates a feeling of confidence. One or two hundred samples can be loaded at once, and the results are neatly tabulated by a typewriter and punched on tape for handling by a computer which may even be included in the package. We are tempted to feel that the automatically printed numbers must indeed represent the absolute truth, but actually our confidence must be carefully established and continually re-established. Neither men nor machines are completely or consistently reliable.'

When considering the counter itself, one initially relied on efficiency (E) and background (B) values as indices of performance and later the so-called figure of merit or E^2/B . If one is working at high count rates, the standard deviation of counting is minimized by using the highest efficiency attainable. If one is working with count rates much closer to background, then E^2/B is a better figure of merit on which to rely.⁹ But if one is interested in dual-label counting, Klein and Eisler have stated that perhaps other figures of merit should be considered.¹⁰ Using varying isotope ratios and channels ratio techniques, they devised separation efficiency numbers (S) which were then used to compute an overall performance number (P) which was the product of the S value and the efficiencies for both isotopes at their point of optimum separation. When published five years ago, they had tested ten instruments representing four manufacturers and the best performance value was one-third of that theoretically attainable. (This P value figure of merit should not be confused with the P value figure of merit discussed by Gibson in Chapter 2 and elsewhere.¹¹ Likewise, the merit value discussed by Fox in Chapter 15 is something completely different from any of the foregoing).

The ultimate in providing us with the best instruments for making our mistakes are the fully-automated systems with built-in computers. As one conjures potential alliance with one of these sleek sirens, consider the comment by Forrey:¹²

'The introduction of tape punch and teletype outputs, automatic external standardization units and internal computers in the counting instruments themselves has raised the question of how best to carry out these calculations most economically, flexibly and conveniently. The equipment manufacturers have not been explicit in the various alternatives available to the user, the cost attendant in each and the details of implementation.'

QUENCHING EFFECTS

Since our biggest common data handling problem is quench correction, let us briefly consider its types and then review the data handling techniques for its determination. If

you prefer to avoid the problem altogether, avoid materials that quench. In this regard, we should not forget that the early literature provides very useful information on common quenching materials. The 1957 paper by Kerr, Hayes, Newton and Ott¹³ is one which lists many of these agents and Dr. Birks has discussed their influence when using counters with the currently available better photomultiplier tubes (see Chapter 1).

In classifying quenching phenomena, the combined approach of Neary and Budd¹⁴ and of Peng¹⁵ is not unreasonable until we have a better classification. We therefore distinguish between chemical, colour and 'photon' quenching. Chemical quenching means the non-fluorescing molecules in the system absorb the β -energy and convert it eventually to heat instead of fluorescence. Such events occur before the emission of photons and the effect is exponential with the concentration of quencher. Colour quench is the attenuation of emitted photons. Since the path length to phototube alters pulse height distribution, this attenuation phenomenon is what distinguishes colour from chemical quench and allows this distinction to be demonstrated experimentally. Peng further distinguishes what is termed 'photon' quenching. Such quenching results from adverse geometry and insolubility phenomena occurring especially in heterogeneous systems. In such systems, the physical mass of dispersed material can prevent β -radiation interaction with the scintillation fluor.

For chemical quenching, a number of subclasses have been proposed. Neary and Budd distinguish between acid, excess fluor concentration, dilution effects, dipole-dipole interaction, and capture of secondary electrons. Those interested are referred to their discussion at the Boston symposium.¹⁴

Quench correction

Krichevsky *et al.*¹⁶ have divided quench correction techniques into direct and indirect types. Direct methods include internal standardization and the extrapolation method of Peng.¹⁵ Channels ratio and external standardization techniques are the indirect types. Although it never became popular for routine use, one could also include the isolated internal standard technique of Ross¹⁷ as a direct method.

Before quench correction became so instrumentally simple and concurrently so mathematically complex, one used the simple formulae of Table 2(a) to calculate d.p.m. After counting the spiked sample, the formulae of Table 2(b) were used to obtain the quench corrected d.p.m. At this point it should be noted that in those early days we all knew what efficiency meant – it was the machine efficiency when a sealed, non-quenched sample of known activity was counted. Anything less was quenching. Today one must be semantically aware since many current quench correction techniques combine efficiency and quenching effects into the single term 'efficiency'. Some might prefer to call this an apparent or relative efficiency.

The discriminator ratio technique^{18,19} was an early method for dual-label counting and quench correction, but still utilized internal standardization. As better multiple channel instruments became available, the pulse height shift with quenching could be determined (see Fig. 1). This led to quench determination by pulse height shift or channels ratio.^{20,21} Baillie spelled out its pros and cons over ten years ago,²⁰ indicating its limitations as:

1. poor overall accuracy with tritium;
2. not usually being useful with strongly quenched coloured samples, and
3. having slightly inferior accuracy for very low level, quenched samples.

He listed advantages as:

Table 2. Primary computations used in programs.

(a) Basic computations

$$\text{Net c.p.m.} = \frac{\text{Total counts of sample}}{\text{Total time of sample}} - \frac{\text{Total counts of background}}{\text{Total time of background}}$$

$$\text{Efficiency} = \frac{\text{Net c.p.m. of standard}}{\text{Known d.p.m. of standard}}$$

$$\text{Net d.p.m.} = \frac{\text{Net c.p.m.}}{\text{Efficiency}}$$

(b) Internal standard quench correction

$$\text{Fraction 'seen'} = \frac{\text{Net d.p.m. with spike} - \text{net d.p.m. without spike}}{\text{d.p.m. of spike}}$$

$$\text{Corrected d.p.m.} = \frac{\text{Net d.p.m. without spike}}{\text{fraction 'seen'}}$$

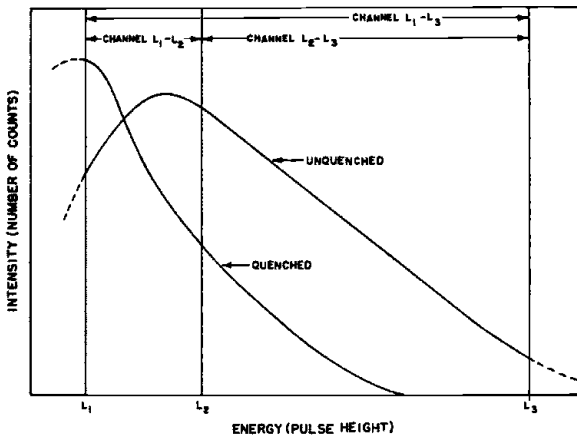


Fig. 1. Spectrometer channels in relation to β -spectra (from Ref. 21).

1. considerable time savings in routine counting;
2. improved accuracy for hot samples;
3. elimination of error due to measurement of standards, and
4. ability to recount samples at a later time since no internal standard had been added.

Five years ago, Rapkin generally concurred with this analysis,²² but countered Baillie's time-saving statement for some by stating that the method:

'..... does have two inter-related limitations which have generally discouraged its use for low-activity samples. When collecting adequate statistics for the channel of principal interest, the count for the weaker channel is apt to be inconclusive. And this situation worsens as quenching increases. In order to collect adequate data for the weaker channel, it is often necessary to count each sample for an excessively long time. This can make the channels ratio technique more time-consuming than the internal standard method.'

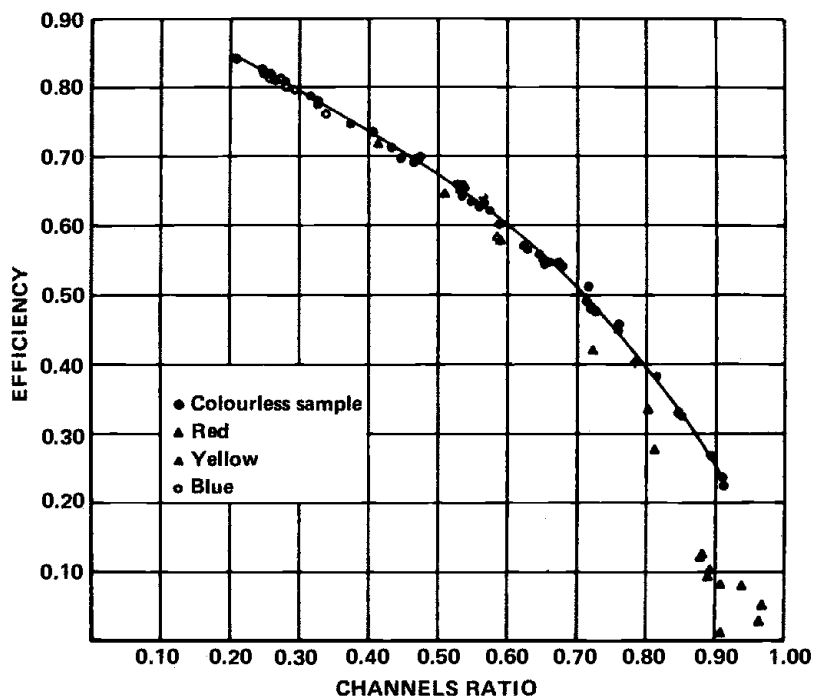


Fig. 2. Quenching curve for carbon-14 using wide channel (L_1-L_3) efficiency versus ratio of counts in channels $(L_1-L_2)/(L_1-L_3)$ (from Ref. 21).

The concern for this method with greater quench and/or low count rates is exemplified in Bush's report²¹ (see Fig. 2). With multiple channel machines where one could independently set upper and lower levels for each channel came a variety of improvements on the technique and it is presently still very useful.

With the advent of automatic external standardization^{23,24} we completed the major spectrometer features grossly evident to the user which have influenced data handling. Additional welcome electronic and mechanical improvements such as markedly improved photomultiplier tubes and circuitry have certainly occurred. However, many recent developments have been more concerned with a plethora of gadgetry to manipulate the count rate obtained rather than the production of the basic count rate. As such, these are developments in the data processing components of the instrumentation rather than in the spectrometer component.

Problems of quench correction for dual-label samples have received attention with many methods promulgated over the years. The early methods included the extrapolation method of Peng²⁵ and the channels ratio methods of Hendler.²⁶ These various techniques have been applied to colour²⁷ and other quench correction problems. The sample channels ratio method of quench correction has afforded Neary and Budd¹⁴ the opportunity to clearly demonstrate that chemical quenching is different from colour quenching (see Figs. 3, 4 and 5).

The phenomenon of different degrees of 'spillover' between channels with varying quench (Fig. 6) is the basis for channels ratio quench correction. When two isotopes are

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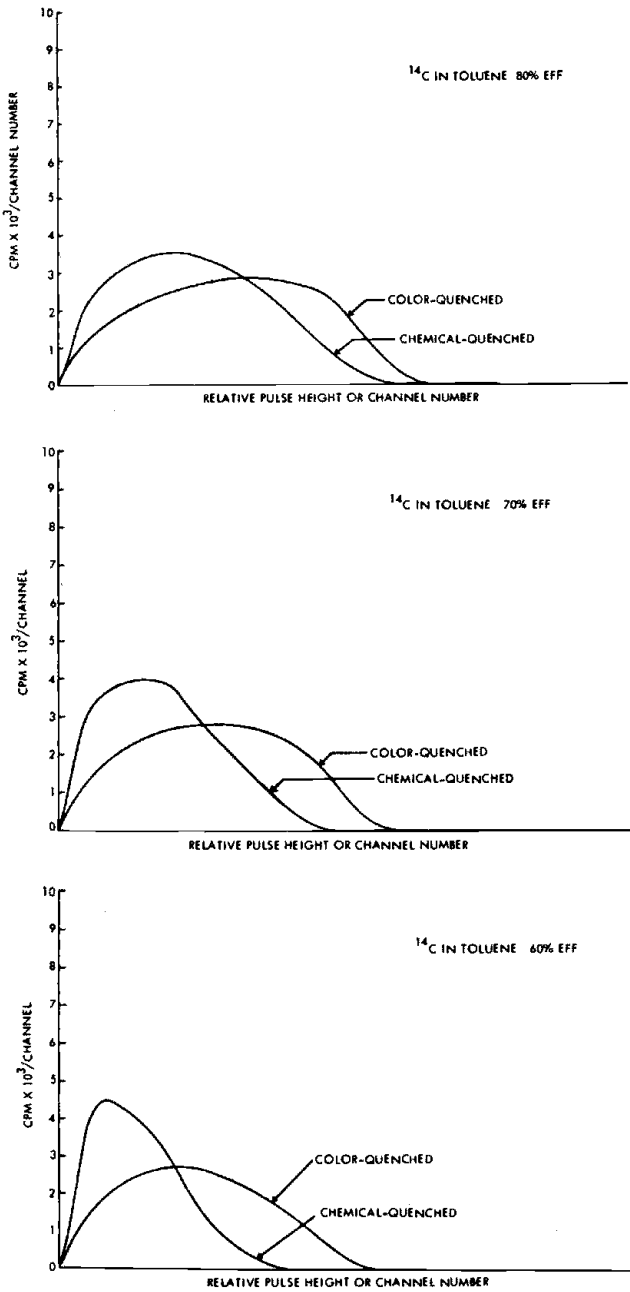


Fig. 3. Colour versus chemical quenching of carbon-14 (from Ref. 14).

used, the formulae for the d.p.m. of both the low energy isotope (D_l) and the high energy isotope (D_h) necessitate the use of five parameters (Table 3). When spillover occurs both ways, one can use the simultaneous equations and Engberg plots discussed by Kobayashi and Maudsley at the Boston symposium.²⁸

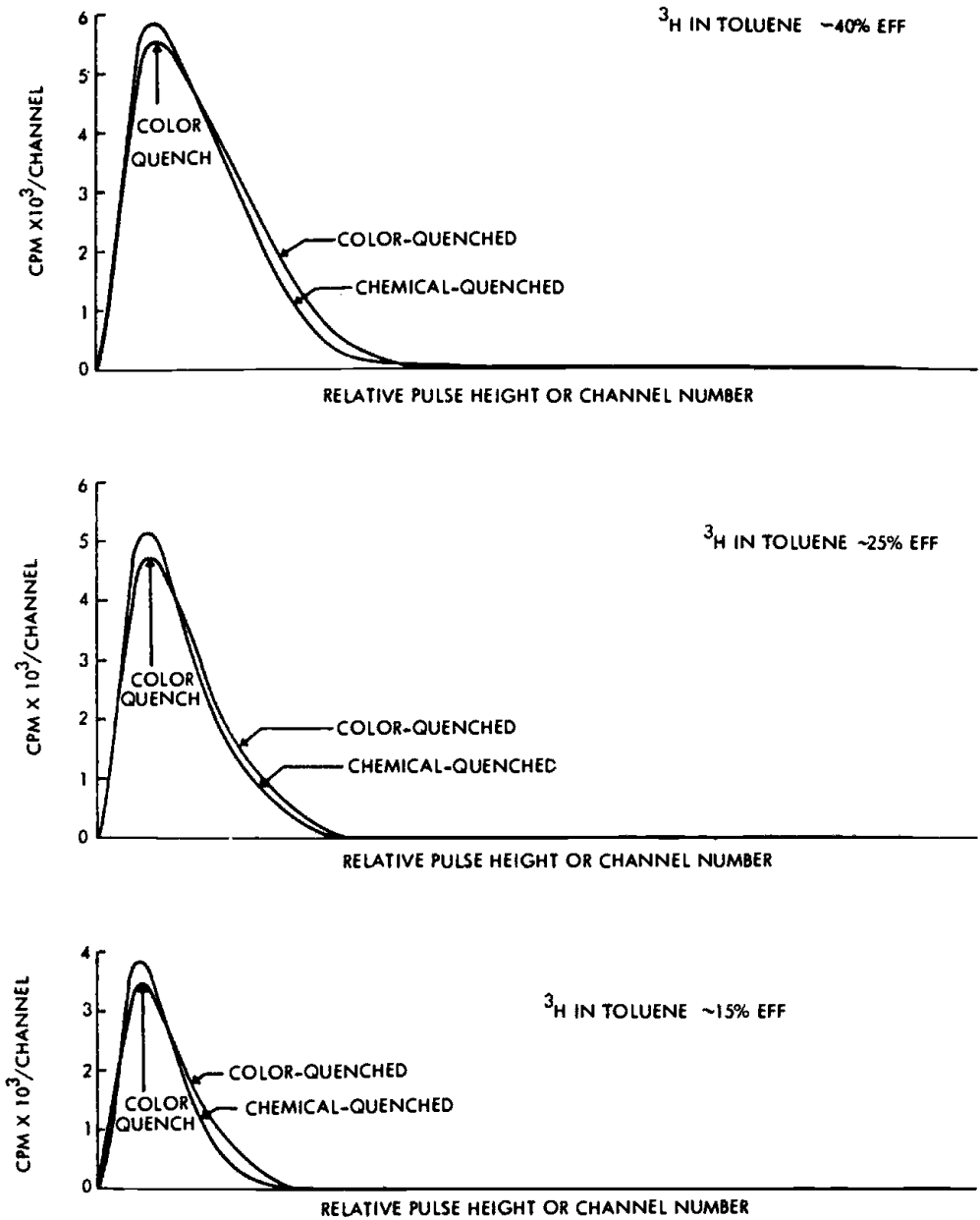


Fig. 4. Colour versus chemical quenching of tritium (from Ref. 14).

Before proceeding further, perhaps another semantic clarification is in order. When channels ratios first came into being, one was referring to the comparison of a discrete lower pulse height channel to that of a higher pulse height channel. This was the original 'sample channels ratio' or 'isotope channels ratio' concept. However, with the introduction of overlapping channels and external standardization, the literature has become more

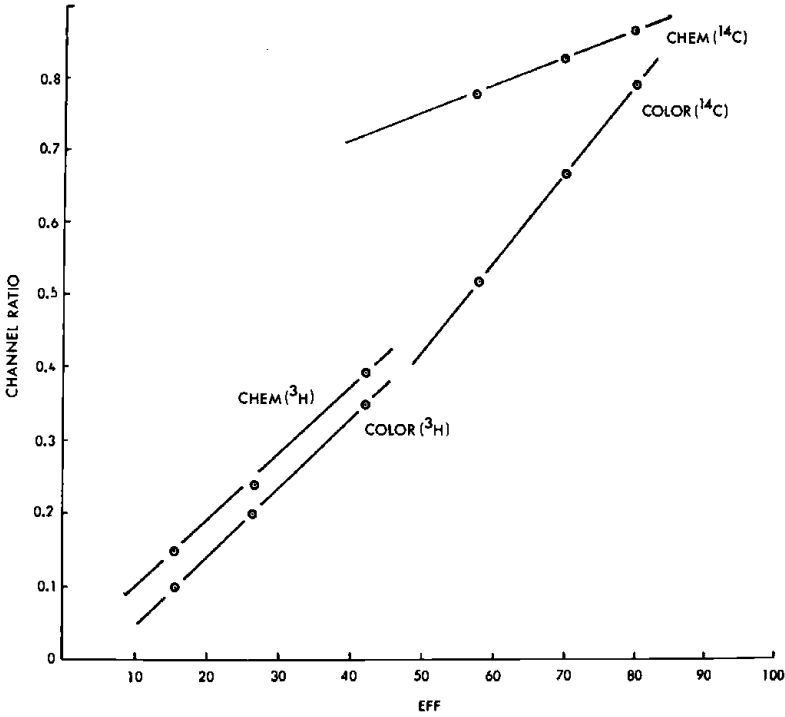


Fig. 5. Effect of differences between chemical and colour quench on quench correction of ¹⁴C- and ³H-toluene samples by channels ratio method (from Ref. 14).

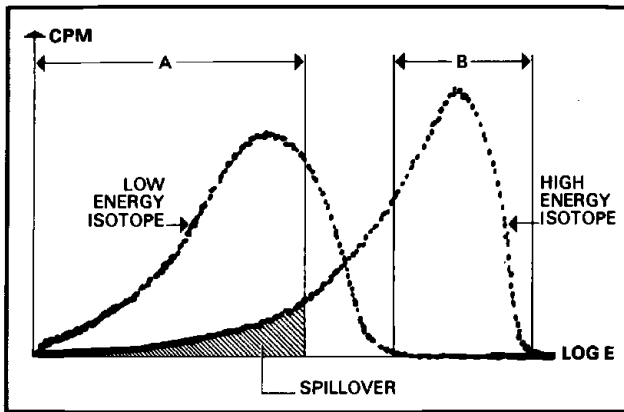


Fig. 6. Spillover of higher energy spectrum in the low energy channel (from Intertechnique brochure No. 12-Multimat-1-10/70).

confusing. Various references to channels ratios may mean sample channels ratios or external standard channels ratios – with or without overlapping pulse heights. This is an unfortunate circumstance and we should all better describe our methods for the sake of clarity.

Not too many detailed comparisons have been made between the more recent methods

Table 3. Dual isotope quench correction with 'spillover' in one direction.^a

C_a	=	count rate low energy channel A including spillover
C_b	=	count rate high energy channel B due to high energy isotope only
E_{hb}	=	efficiency of high energy isotope in high energy channel B
E_{ha}	=	efficiency of high energy spillover in low energy channel A
E_{la}	=	efficiency of low energy isotope in low energy channel A
D_l	=	$\frac{C_a - C_b(E_{ha}/E_{hb})}{E_{la}} \equiv$ d.p.m. of low energy isotope
D_h	=	$\frac{C_b}{E_{hb}} =$ d.p.m. of high energy isotope

^a After Intertechnique Brochure No. 12-MultiMat-1-10/70

of quench correction. However, when such comparisons have been made, the results have been illuminating. Noujaim *et al.* have compared automatic external standardization to channels ratio techniques.²⁹ They concluded that with instrumentation available a year ago the sample (or isotope) channels ratio method is quite satisfactory for reasonable counting rates with colour quenched samples. However, they found automatic external standardization (AES) correlation or external standard ratios much less satisfactory. This was true for both tritium (Fig. 7) and carbon-14 (Fig. 8).

The empirical approach on the differentiation between colour and chemical quench by Lang³⁰ may be of particular interest to many. He has devised a system whereby one may discriminate between colour and chemical quench on a *post hoc* basis. He has found that chemical quench and colour quench are different when apparent efficiency are plotted against the square root of the AES c.p.m. or against the AES channels ratio (Fig. 9). In his presentation at the San Francisco symposium he goes on to demonstrate how a sample may be adjudged to be chemically quenched or colour quenched by comparing its counting performance for apparent efficiency using these two correlations.³⁰

It is also interesting to note that while we pay homage to the recent methods, Rogers and Moran compared internal standardization, external standardization, and sample channels ratio methods of quench correction³¹ and stated that:

'The careful addition of internal standard is shown to give the highest accuracy in determination of the efficiency of liquid scintillation counting. The technique of channels ratio is equally accurate, when used with samples that are moderately quenched and have a high counting rate, and less accurate for highly quenched samples. Automatic external standardization is considerably less accurate than either of the other techniques.'

The necessary conclusion to be drawn from these limited comparative studies is that there is no recommended universal quench correction technique. They are all useful as long as one operates within the boundary conditions of the respective methods.

STATISTICS

Counting statistics is an obviously important consideration in data handling. Graphs, nomographs and mathematical treatments appear throughout the literature and in commercial material. Still useful early sources include those of Jarrett,³² Loevinger and Berman,³³ and Browning.³⁴ The questions associated with single isotope counting versus dual isotope counting have respectively been considered by Herberg³⁵ and by Bush.³⁶ The

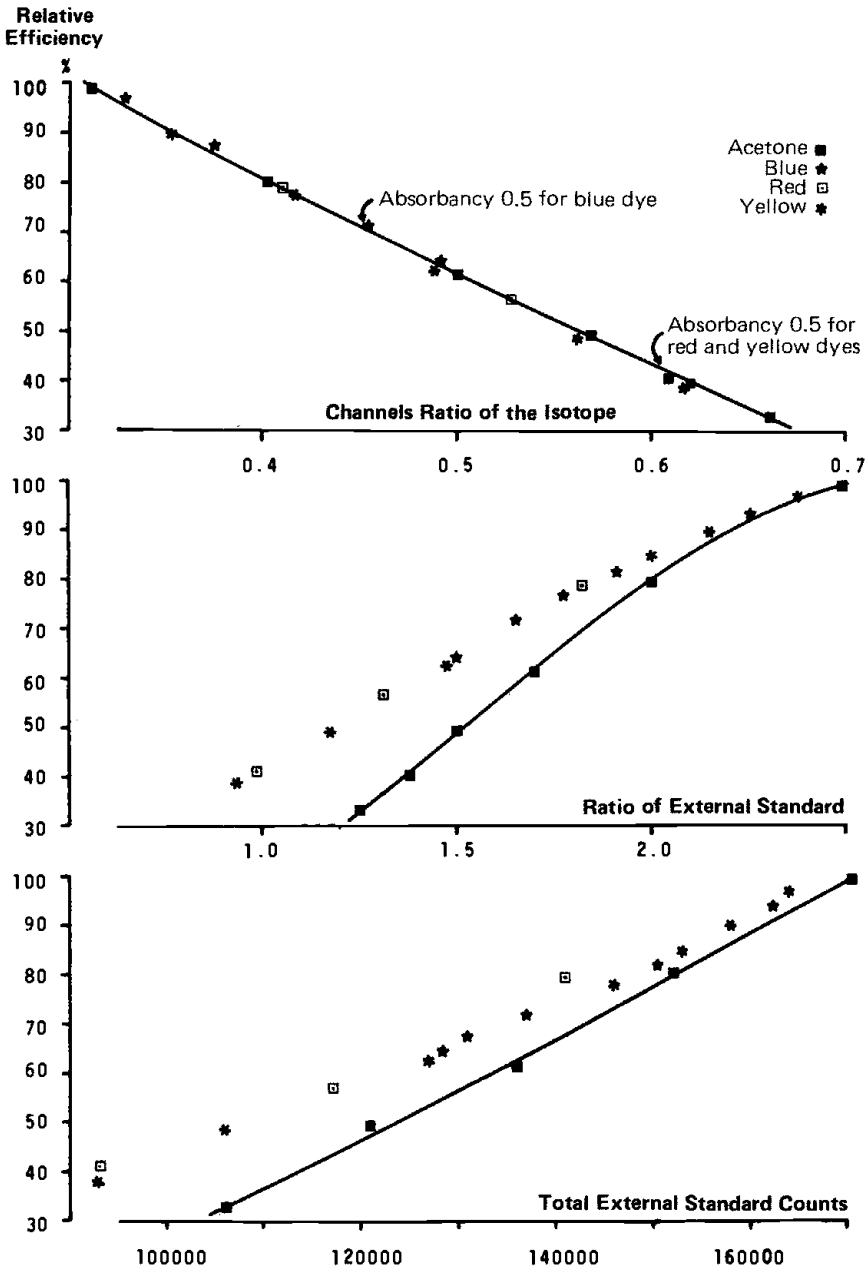


Fig. 7. Counting efficiency correction curves for tritium (from Ref. 29).

question of whether one should accept the Poisson model for estimation of counting error has been discussed by many, including Matthijssen and Goldzieher,³⁷ Cavanaugh³⁸ and Carroll and Houser.³⁹ In testing the Poisson model, where the square root of the count is the error of that count, Matthijssen and Goldzieher concluded that liquid scintillation spectrometers were not stable enough to support the assumption of conformance with

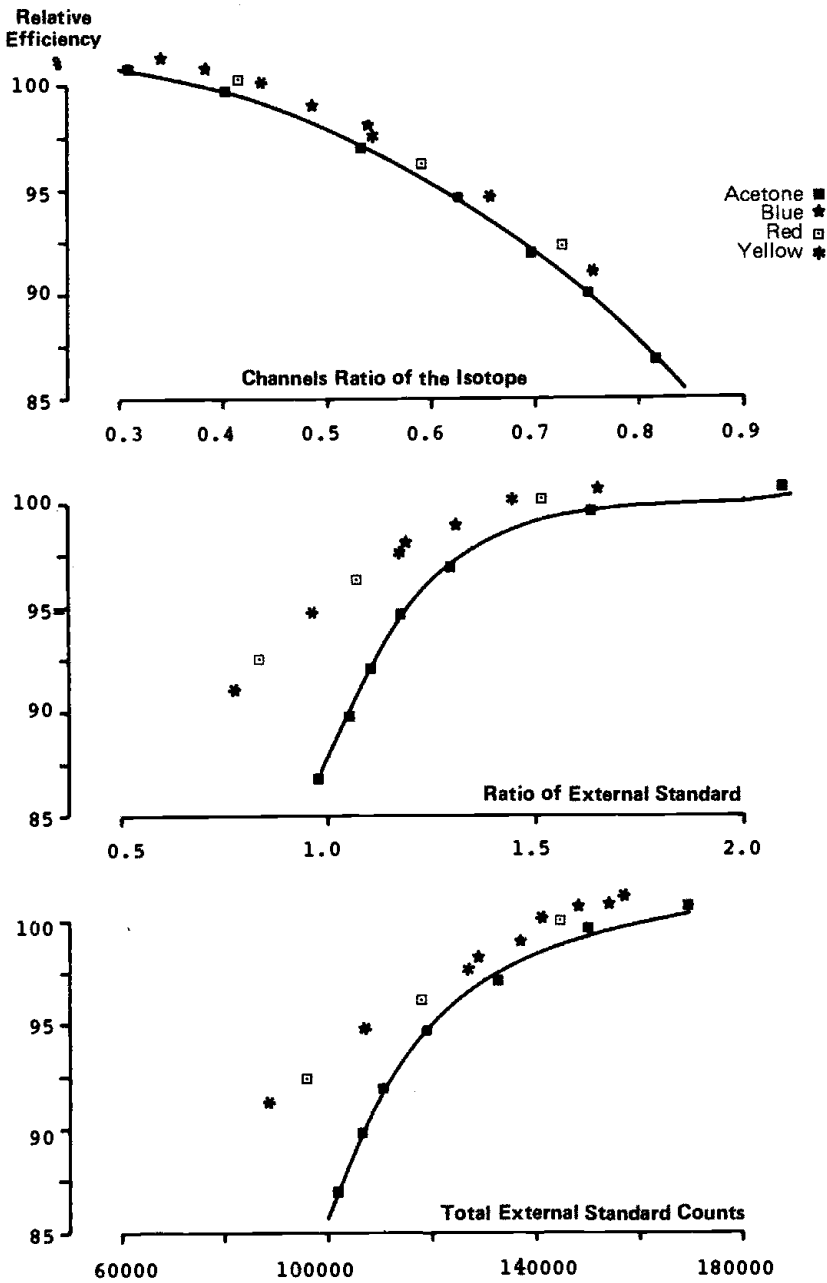


Fig. 8. Counting efficiency correction curves for carbon-14 (from Ref. 29).

the Poisson binomial distribution model.³⁷ This led them to state that chi-square is inappropriate for measuring instrument stability and they recommended the relative standard error instead. In discussing the statistics of external standardization methods, Cavanaugh recommends use of external standard ratios rather than the external standard counts *per se*

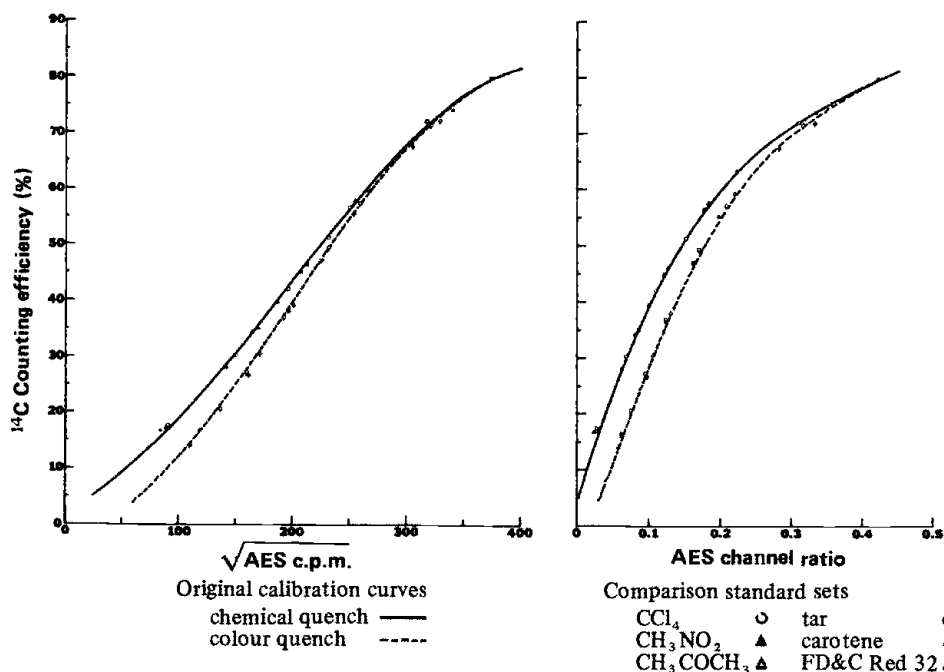


Fig. 9. Comparison of various quenching agents on carbon-14 chemical and colour quench calibration curves (from Ref. 30).

since the ratio technique quench correction curves are less dependent on volume.³⁸ Cavanaugh also states that averaging of sample counts from different counting cycles helps reduce non-Poisson errors.

COMPUTER PROGRAMS

In turning to the subject of computer handling of data, it was obvious quite early that liquid scintillation counting was becoming so automated that the necessary mathematical manipulation of the counts obtained was becoming the bottleneck. At the present time there is no way of knowing how many computer programs are available for such computations. The programs by Blanchard,⁴⁰ Spratt,⁴¹ and Axelrod *et al.*⁴² were among the early ones reported in the literature. Many more have subsequently appeared including an external standardization update of our program.⁴³ Spectrometer manufacturers have also collected an additional number of programs not necessarily described in scientific journals.

Quench techniques used in the many programs now described include internal standardization,^{40,41} discriminator ratios,⁴⁴ sample channels ratios,^{12,16,39,42,45,46} external standardization,^{12,30,42,43,47,48} and external standard ratios.^{12,30,39,45,46,48-50} Quench correction for dual isotopes in the same sample are available in many of these programs.^{12,16,39,44,46,48-50} Most are used on relatively large computers, but some are designed for smaller programmable calculators or computers.^{45,46,48,50} Throughout these various programs one often finds that the correlation of the quench parameter is not linear with the apparent efficiency. For this reason, a polynomial expansion to an appropriate power is often used.

The program described by Glass⁴⁵ is of particular note since all samples are quench

corrected by both the sample channels ratio technique and the external standard ratio technique. This double ratio method allows for the *post hoc* selection of the most appropriate of the two quench correction techniques for each sample. In addition, it also permits a number of discrepancy checks on both the samples and the counter.

The literature describing these programs contains various comments on the question of on-line versus off-line computation.^{46,48,51,52} However, whenever such comparisons are made, it must be recognized that the comparison is only valid when examined in respect to the individual user's environment. For example, Moore's comparison⁵¹ of batch processing versus time-sharing obviously considers a number of local features. It also mixes programming concerns with production run concerns.

The instrument manufacturers are still continuing with their own gadgetry modifications which are sold as instrumentation specifically wedded to their own spectrometers. Among these modifications are the Packard Absolute Activity Analyzer and the Multi-Mat system recently announced by Intertechnique. Although the commercial literature on both of these systems refers to their ability to determine 'absolute activity', the activity of any counter should be just as 'absolute' when properly determined.

The Packard Absolute Activity Analyzer operates by defocusing the photomultiplier tubes for each unknown sample so that the external standard ratio for each sample will be identical to that of one of the previously determined ratios for a set of sealed standards.⁷ The refocusing step may be repeated up to fifteen times if necessary. When the sample counting conditions match one of the standard points, the sample is counted and the d.p.m. computed. Two sources of comments on the Absolute Activity Analyzer are the presentation by Cavanaugh of Packard³⁸ and the independent evaluation by Herberg.⁵³ It should be noted that the Beckman 'Automatic Quench Correction' takes a related but somewhat different approach by the readjustment of system gain via varying amplification.⁷

From the commercial literature available, it appears that the Intertechnique Multi-Mat system involves the concurrent purchase of a small on-line computer which performs the usual quench corrections from curves which can be stored in its computer. This is the same approach that has been used both on-line and off-line by many investigators. The Multi-Mat system is somewhat different in that the on-line computer processing unit can simultaneously accept counting data from up to four spectrometers within 300 ft of the processor. This system also incorporates the feature of computing the net count error as opposed to the gross count error (Table 4). A useful discussion of the 2σ error has been provided by Wyld.⁹

Throughout all of the foregoing discussion it has been apparent that we now have all kinds of ways of handling our liquid scintillation counting data. However, we should never blindly rely on a count present 'in living colour' on nixie tubes or crisply printed in beautiful alignment by a computer. What went into the laboratory manipulations and the preparation of the sample must always be considered. Some potential pitfalls might arbitrarily be considered as sample factors, counter factors, and calculator/computer factors.

Sample factors

Sample factors (Table 5) include the vial cap and the vial itself in regard to physical composition, isotope composition, and regularity of its walls. The peroxides in dioxane and impurities in other solvents are of concern. The miscibility of the solvents at the counting temperature should, of course, be noted. When suspension systems are used, one must

Table 4. Gross versus net count rate error.^a

(a) Measurements	
S	= gross sample count rate
B	= background rate
t_s	= sample counting time
t_b	= background counting time
(b) 2σ gross count rate error	
$2\sigma_g$ in %	$= \frac{200}{\sqrt{S \times t_s}}$
(c) 2σ net count rate error	
$2\sigma_n$ in %	$= \frac{200 \sqrt{\frac{S}{t_s} + \frac{B}{t_b}}}{S - B}$

^a After Intertechnique brochure No. 12-MultiMat-1-10/70.

Table 5. Sample factors

Counting vial
Solvents
Miscible system
Volume
Phosphor and wavelength shifter
Chemical reactions
Volatilization
Precipitation
Fluorescence (dark adaptation)
Aberrant environmental background
Temperature (equilibration and condensation)

also consider uniformity of dispersion and the problems of potential self absorption or 'photon' quenching. Newer instrumentation includes light pipes, compound external standards and other features which minimize volume problems. However, these features are not on many counters still in use.

As mentioned earlier, excess fluor components can surprisingly cause quenching¹⁴ whereas too little fluor or improper balance between primary fluors and wavelength shifters can result in less than optimal efficiency.

Chemical reactions between components in the sample are possible, as are volatilization or precipitation of constituents. These types of phenomena, as well as fluorescence from non-radioactive components⁵⁴ can sometimes be detected by multiple cycle counting of the same sample.

One should also not have tunnel vision in regard to environmental factors. Background is not a feature of sample and counter performance alone. Although stabilized by shielding and spectrometer electronics, it can still be influenced by radiation in the area. The temperature of the sample preparation area and the temperature during counting is another important environmental consideration. The sample should always be equilibrated to the counting temperature to minimize condensation, unanticipated precipitation, and other problems.

Table 6. Counter factors.

Photomultiplier tubes
Mechanical failure
Circuitry failure
Power failure
Positioning of AES pellet
Aberrant event (i.e. dead fly)

Counter factors

Temperature is important in counter factors as well (Table 6), especially in relation to the type of photomultiplier tubes. Mechanical and circuitry failure is to be expected with anything as complex as today's liquid scintillation spectrometers. If the event is a complete and obvious malfunction, it is often less frustrating than the intermittent, less readily detected malfunction. The same can be said for line voltage problems in the building's electrical supply. Various protective devices have been incorporated to minimize detrimental counter effects in the event of total power failure. However, power problems for both the spectrometer and the necessary air conditioning can be a constant source of concern.

A specific electro-mechanical malfunction can be the improper positioning of the external standard pellet, especially on a non-predictable basis.

My favourite malfunction concern for any instrumentation is the completely non-predictable, intermittent aberrant event which might be called the 'dead fly' or the 'grey hair' factor. This usually happens when one has a critical experiment going or needs another replicate experiment to complete the statistical comparisons in a paper to be presented the next week for which the slides have already been made. On the other hand, it never demonstrates itself when the service man is in attendance or when the counter is not being heavily used. The eventual explanation — if any — is often a dead fly or moth, some dust or lint, an old spider web, or some similar item to remind us of our complete subservience to the whims of nature.

Calculator/computer factors

If the sample has perchance miraculously survived all of the aforementioned pitfalls, you now have a count. However, this count is still subject to calculator/computer factors (Table 7) — whether on-line or off-line — before it becomes a useful datum. Electro-mechanical events and power problems can play a role, just as they do with the spectrometers. One of the favourite foibles of these devices is to print or punch an extra digit or

Table 7. Calculator/computer factors.

Circuitry failure
Mechanical failure
Power failure
Lack of parameter checks (i.e. precise nonsense)

one less digit just to be different on occasion. If enough appropriate checks on the system are not utilized, this kind of event can produce well-formatted, beautifully typed sheets essentially ready for publication — except that the figures are nonsense!

Calculator/computer selection

In deciding what hardware route to pursue for liquid scintillation data handling, the first step appears to be self-evident. Except in those circumstances where only an occasional sample is counted or samples of known quench are put through a simple screening procedure for one fixed level of radioactivity, everyone is or will be using programmable calculators or computers. Quite frankly, the experiment generating the samples often has an error which deserves only slide-rule precision and we should therefore always be acutely aware of the number of significant figures we are dealing with when using various automatic computational devices. On the other hand, as I stated earlier, with the currently available multi-sample automatic spectrometers, the main bottleneck at the moment is data handling. As such, the remaining question is what direction one takes in regard to utilizing a programmable calculator, a mini-computer or a large computer. Recent developments in programmable calculators and mini-computers are making them more competitive with large computers and therefore such decisions must always be made in the investigator's local environment with the most recent information available.

Table 8. Considerations in calculator/computer selection.

Dedicated	versus non-dedicated
Unique run	versus production run
Single count	versus count averaging
Off-line	versus on-line
Batch process	versus time sharing
Turn around time	versus cost
Machine readability	versus hard copy only
Laboratory	versus institutional considerations

The individual investigator (and possibly others) must consider whether the convenience of data reduction from the liquid scintillation spectrometer may be worth the price of a computation device devoted to this exercise (dedicated) or whether this is a more centralized computer problem (non-dedicated) (see Table 8). One must also consider the uniqueness of the experiments. If one is doing only one experiment it may not be worth getting involved in computer programming. But if one is anticipating routine production runs of data after the program has been established, the computer approach may be completely satisfactory.

The question of count averaging has already been alluded to earlier where it was mentioned that Cavanaugh has shown that averaging can improve counting statistics.³⁸ In terms of instrumentation, such averaging is obviously handled off-line.

Off-line versus on-line is very much a local decision. The price of the gear associated with the spectrometer and the off-line local capabilities need to be considered. No one has a specific answer for these considerations except those immediately involved. Batch processing versus time sharing is also very much a local consideration, depending on the available facilities.

Turn around time is always a sticky consideration. Everyone wants immediate turn around time but very seldom do we really need this immediate turn around. The one exception is the necessity for real-time interaction such as in physiological experiments where computation will immediately influence the subsequent experimental parameters. Such needs are seldom, if ever, present in liquid scintillation spectrometry. As such, except in a possible rare circumstance of flow-through analysis, this has to be considered as a moot point. However, one must also remember that other moot points can have very real and very meaningful importance to very real individual investigators who have anticipation deadlines.

The potential cost of opting for fast turn around time has of course had an effect on many investigators. Whether one is considering operating on-line or off-line, the potential is there if one is ready and willing to pay for fast turn around.

Table 9. Advantages of machine readability.

Editing capabilities
Data storage
Data transformation
Data display
Ready statistical analysis

When one considers machine readability, a number of considerations come to mind -- some of which do not always present themselves when the raw data is computed (see Table 9). Once the data are machine readable, appropriate program steps can interrogate the data to assure that input and output errors have not been made and various manipulative procedures on the data can also be performed. These options are in distinct contrast to a fixed program facility where only a hard copy with a fixed format is available.

Before concluding this presentation, it is only appropriate to recognize that the needs of a given individual investigator may not necessarily completely agree with other investigators in a given institution or the institution at large. This last stated consideration is not necessarily the least of our concerns. Everyone wants his or her own institution to flourish and yet everyone wants to do his or her own thing. As such, this consideration must be adjudged by us all, both individually and collectively. The environments and the solutions may be different, but the considerations are reasonably common to all.

In concluding, I realize that I have been variously repetitious of prior speakers and have perhaps covered too much. However, I hope this overview has set the stage for the more specific presentations to follow and, in assembling various user concerns, that it will prove beneficial for both current and future users of liquid scintillation spectrometry.

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DISCUSSION

E. Rapkin: I have two comments to make; firstly the Intertechnique counters are capable of storing repetitive counts and averaging results. Also, those Intertechnique counters which are capable of computing d.p.m. can average results of repetitive computations, thereby effectively averaging results of repetitive external standardization.

Secondly, too many users trust d.p.m. values based on calibration curves constructed from a single external standard count (30 s in/30 s out) and then a single external standard count of their test samples.

J. L. Spratt: In regard to your first point, once the first cycle count has been determined and stored, one is operating off-line in regard to further data processing of that number. This is true whether the computer facility sits on the counter or is a detached computer some distance away. Either way, I always appreciate having the option of multiple cycle counting and data handling which you mention.

Your second point is a quite valid concern for all of us.

J. H. Deterding: Would you like to comment on what is to me, the surprisingly uncritical acceptance of the performance number of P. D. Klein and W. J. Eisler (*Anal. Chem.* **38**, 1453 (1966))? I believe that there may be alternative, less arbitrary, criteria for the comparison of the performance of instruments used in experiments involving the counting of two isotopes.

J. L. Spratt: I share your concern on how much reliability we should place on Klein and Eisler's performance numbers. However, their approach was mentioned for the sake of completeness and to indicate that instrument performance can be viewed in many ways, depending on the instrument's use. They may be criticized for being somewhat arbitrary, but they cannot be faulted for at least attempting to devise criteria other than efficiency (E), background (B) and E^2/B .

J. L. Spratt: Comment: From various concerns expressed elsewhere at these meetings, perhaps it is appropriate for us to return to a dissociation between the counter and the sample in reference to efficiency. Both the manufacturers and users would then be in a better position to debate the relative merits of the basic instrumentation versus the uses to which it is put.