QUENCH: A Software Package for the Determination of Quenching Curves in Liquid Scintillation Counting

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In Liquid Scintillation Counting (LSC), the scintillating source is part of the measurement system and its detection efficiency varies with the scintillator used, the vial, the volume and the chemistry of the sample. The detection efficiency, ε, is generally determined using a quenching curve, describing, for a specific radionuclide, the relationship between ε and a quenching index, *QE*, given by the counter. A quenched set of LS standard sources are prepared by adding a quenching agent and *QE* and ε are determined for each source. Then a simple formula is fitted to these experimental points to define the quenching curve function. This poster describes a software package specifically devoted to the determination of quenching curves with the uncertainties. The experimental measurements are described by their quenching index and detection efficiency with uncertainties on both quantities. Random Gaussian fluctuations of these experimental measurements are sampled and a polynomial or logarithmic function is fitted on each fluctuation by χ^2 minimization. This Monte Carlo procedure is repeated many times and eventually the arithmetic mean and the experimental standard deviation of each parameter are calculated, together with the covariances between these parameters. Using these parameters, the detection efficiency, corresponding to an arbitrary quenching index within the measured range, can be calculated. The associated uncertainty is calculated with the law of propagation of variances, including the covariance terms. In parallel, the uncertainties of the quenching curves are also estimated directly by a Monte Carlo method without using the law of propagation of variances.

Method

Experimental data:
- Quenching index, *QE* and u_{QE}
- Experimental detection efficiency, ε and u_ε
- Uncertainty on the activity of the radionuclide standard, u_A

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- *n* Gaussian fluctuations of each experimental point
- Uncorrelated fluctuations of *QE* and ε
- Additional correlated fluctuations for each ε to take u_A into account

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Fitting function, e.g. $\varepsilon = a_1 + a_2QE + a_3QE^2 + \ldots + a_nQE^{n-1}$
Iterative fitting process with *n* sets of points

→ *n* values of the a_i parameters of the fitting function

GUM supplement 1 approach

Calculation of *n* values of ε and calculation of the mean value of ε with associated experimental standard deviation u_ε

Mean and experimental covariance matrix of the a_i parameters

Experimental QE value

Calculation of ε with the mean parameters of the function of fit

Calculation of u_ε with the covariance matrix (sum of the experimental covariance matrix from the *n* repetitions and the covariance matrix of the fit process), using the law of propagation of variances

GUM approach

Algorithms

Random number generation

Uniform deviate: period > $2 \cdot 10^8$

Gaussian deviates: transformation method

Maximum likelihood criterion

χ^2 minimization (maximum likelihood criterion for Gaussian fluctuations)

Minimization algorithm

Levenberg-Marquardt

Automatic adjustment of the number of parameters

Fitting functions

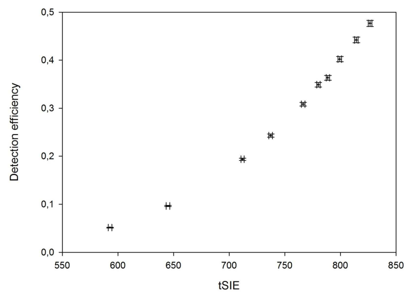
Polynomial
$\varepsilon = a_1 + a_2QE + a_3QE^2 + \ldots + a_nQE^{n-1}$

Logarithmic
$\varepsilon = a_1 + a_2 \ln(QE)$

Programming toolbox used: Numerical Recipes, 3rd edition. W. H. Press, S. A. Teukolsky, W. T. Vetterling, B. P. Flannery. Cambridge University Press, 2007.

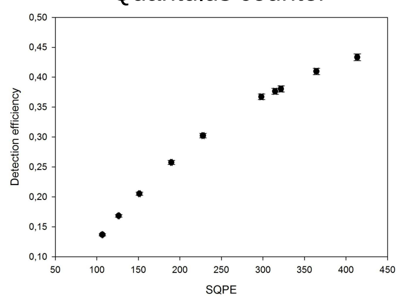
Example of calculations for tritium

TriCarb counter



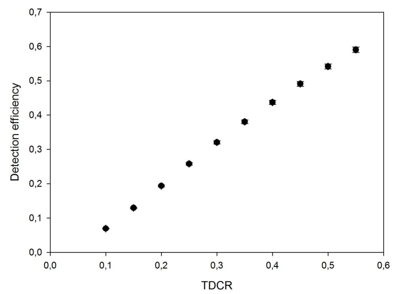
For *tSiE* = 350, 4th order polynomial
With only u_ε, ε = 40.51 (13)
With u_ε and u_{tSIE}, ε = 39.99 (63)
With u_ε and u_{tSIE} Monte Carlo, ε = 39.99 (62)

Quantulus counter



For *SQPE* = 750, 4th order polynomial
With only u_ε, ε = 27.56 (8)
With u_ε and u_{SQPE}, ε = 27.13 (46)
With u_ε and u_{SQPE} Monte Carlo, ε = 27.13 (45)

TDCR counter



For *TDCR* = 0.35, 2nd order polynomial
With only u_ε, ε = 37.69 (10)
With u_ε and u_{TDCR}, ε = 37.55 (14)
With u_ε and u_{TDCR} Monte Carlo, ε = 37.55 (10)

→ Underestimation of interpolation uncertainties when not considering the uncertainty of the quenching index

Conclusion

The program "QUENCH" allows the interpolation of quenching curves in LSC. Uncertainties on the quenching index and on the detection efficiency of each experimental point of the quenching curve are considered. The fitting function can be a polynomial or a logarithmic function. The best estimate of the parameters of the fitting function, together with their covariance matrix is calculated. All this information is used to calculate the detection efficiency corresponding to a value of the quenching and its associated standard uncertainty. A full Monte Carlo uncertainty calculation is also provided. The program is freely available on the LNHB web site with a short user guide: http://www.nucleide.org/ICRM_LSC_WG/icrmsoftware.htm

Le progrès, une passion à partager

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