Dosimeter Batch Calibration "Curve Fit" Analysis

GEX Doc #100-215

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SCOPE

GEX regression analysis (curve fitting) of calibration data sets for customers using the Terastat "Calibrate!" software program.

PURPOSE

This document provides an explanation of the process of how GEX analyzes customer calibration data and also explains the statistical tests that are performed on the curve fitting data. This document should help customers to develop some acceptance criteria for their internal procedures, and serves as a reference for future questions that may arise.

METHOD

Data Set Preparation and Review:
GEX staff reviews customer provided dosimeter measurement data and the calibration laboratory certificate for general completion upon receipt from the customers. The completed data sets are evaluated by determining a mean, standard deviation, and coefficient of variation to verify that data sets satisfy specified precision requirements, and for the identification of any potential outlier data prior to undertaking the curve fitting process. In addition, the data sets are plotted and evaluated to verify that the response plot is appropriate based on the expectations for a particular dosimeter and dosimetry system.

Curve Fitting:
GEX utilizes the Terastat "Calibrate!" software program to perform regression analysis (curve fitting) of calibration data sets in order to derive mathematical response functions used to estimate dose from a measured response value. Response functions are generated for each set of measurement instruments and/or instrument data in combination.

The "Calibrate!" software used by GEX was developed by Terastat specifically for use in performing calibration of dosimetry systems and operates as an "add-in" to the Microsoft Excel spreadsheet software program. The software program performs curve-fitting and fit analysis of the calibration data sets by using built-in MS Excel functions.

The "Calibrate!" software performs regression analysis curve fitting of dosimeter response as a function of dose, performing up to five simultaneous curve fits of the data (dependent on the quantity of dose levels).

- Log-linear
- Linear (1st order)
- Quadratic (2nd Order)
- Cubic (3rd Order)
- Quartic (4th Order)

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Individual equations derived for each curve fit along with statistical analysis of fit are provided for review and evaluation by the customer. Analysis of fit involves evaluation of the difference between values derived from the regression model against actual values.

This software compares the fit analysis results of all the generated response functions and determines a "best fit" response function based on internal software criteria.

Goodness of Fit Testing:
The "Calibrate!" software provides a series of statistical analyses, outputs a quantitative evaluation of each fit, and displays the results for each. The results are used by GEX to determine the best fit using the lowest order possible. Meaning, if two results are similar, the lowest order fit will be selected over the higher order fit. The calculated values are used as the primary analysis to determine the best-fit function.

The items that are calculated for each fit are:

- **r-Square:** value from the regression equation used to fit the data. It can be read as the fraction of variability in the response due to changes in the standard value. Often, r-square will be 0.990 or greater and is not a sensitive analysis statistic for determining the best fit. It is displayed because it is a standard type of analysis typically evaluated but is not used to determine goodness of fit for dosimetry system response functions.

- **Regression F Statistic:** the F value of the regression equation. A larger F statistic value indicates the model fits the data well. Often the highest F statistic indicates the best fit and will often track with the lowest MDL although there are exceptions.

- **Significance of Regression:** probability that the observed regression F statistic may have occurred by chance. For almost all calibrations, the p-value will be near zero.

- **Lack of Fit F Statistic:** the F-value of the lack of fit component of the residual variability. This statistic is used to evaluate whether a better fit to the data can be obtained by using a higher order polynomial. The lowest value typically indicates that a higher order fit is not better.

- **Lack of Fit Significance:** probability that the observed lack of fit F statistic may have occurred by chance. If this value is less than or equal to 0.05 ($p <= 0.05$), then the software decides that the lack of fit is not significant. Any value higher than 0.05 will disqualify the fit from consideration as "best".

- **MSE:** Mean Square Error - the variability remaining after fitting the regression equation. The lowest value is typically best.

- **Estimated MDL at 95% confidence:** a calculated "method detection limit" for the fit. This is the value that can be reliably distinguished from zero, and is a major determining factor used in determining best fit. The lower the value, typically the better the fit. It is a function of the total uncertainty of the curve fit and the specified prediction limits.

Plot of Residuals Analysis:

The "Calibrate!" software also provides a plot of residuals that is used for qualitative verification of the "best fit" regression model. The residuals plot is an invaluable tool used to verify the quality of fit of the selected response function. Residual plots should demonstrate generally distributed results around zero without a detectable pattern, which is reviewed by trained GEX technical staff conducting the calibration for the customer. Residual plots also provide a means to verify absence of outlier data that should have been resolved prior to determination of the best curve fit.

Determining the Usable Dose Range of the Selected Response Function:

Once the "best fit" curve has been determined, the "Calibrate!" software is used by trained GEX staff to create a table of dose values covering the calibrated range derived from the calibration response function. The software estimates a dose for each designated response value, and also generates 95% lower and upper prediction limit values for each dose.

A percent uncertainty value with a 95% confidence level is calculated for each dose estimate value using these prediction limits *(upper prediction limit - lower prediction limit) / (2 * dose estimate * 100)*. The uncertainty limits can be used to select the minimum and maximum allowable dose limits of the calibration using a maximum allowable uncertainty value.

Determining the Uncertainty of the Calibration Curve:

Once the calibration curve dose range limits have been established, a median or average value for the usable portion of the calibration range can be calculated. This 'Type A' calibration uncertainty aggregate captures the measurement variability and uncertainty in the fitting. The overall calibration uncertainty is determined by adding the all additional components (Type A and/or Type B) in quadrature. Please refer to GEX Technical Memo 100-209 for discussion and ISO/ASTM 51707 for guidance, see References section below.

LIMITATIONS/PRECAUTIONS

Regarding curve fitting and "best-fit", it should be noted that the customer or GEX can select a different fit based on personal analysis of the residuals plot provided that the resulting uncertainty for the dosimetry system calibration are acceptable to the end-user.

REFERENCES

References:

- *ISO/ASTM 51707: Standard Guide for Estimation of Measurement Uncertainty in Dosimetry for Radiation Processing*
- *GEX Technical Information and Usage Report (TIR) #100-209, Developing and Using Uncertainty Statements*

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REVISION CONTROL HISTORY

DATE	CHANGE DESCRIPTION	REVISION
12/13/16	Initial release.	A
07/08/18	Updated 'goodness of fit' section per ECO 70384.	B

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