Designation: D7510 – 10 (Reapproved 2016)ε1

Standard Practice for Performing Detection and Quantitation Estimation and Data Assessment Utilizing DQCALC Software, based on ASTM Practices D6091 and D6512 of Committee D19 on Water[1,2]

This standard is issued under the fixed designation D7510; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

ε[1] NOTE—Reapproved with editorial change to 4.2.3 in December 2016.

1. Scope

1.1 This software was developed to automate calculations within three ASTM standards: Practices D2777 (outlier removal section), D6091, and D6512.

1.2 The program calculates detection estimates (DE) and quantitation estimates (QE) for the constant, straight-line, exponential, and hybrid (Rocke-Lorenzato) models of the variation of [inter or intra] laboratory standard deviation (ILSD) with concentration. Calculations are shown in the DE_QE worksheet and results are shown in the DLs & QLs worksheet. Several plots are generated showing how well each model fits the data. The least complex model to fit the data with adequate confidence must be used by the ASTM standards.

NOTE 1—Modeling techniques automated in this practice and with this software have been shown to work well with most data sets. Users of this software are cautioned that with some, rare data sets, anomalous results may be obtained, and manual forcing of a different model may be required. It has been noted that for some data sets when an exponential model is selected, there may be a lack of convergence on a result or there may be a convergence on two separate results.

1.3 Users of DQCALC should refer to Practices D2777, D6091, and D6512 for the specifics of the scope and application of the Practices.

1.4 The IDE Practice (D6091) and the IQE Practice (D6512) are concerned with estimates of limits of detection and limits of quantitation based on inter-laboratory data. DQCALC may also be employed to calculate detection and quantitation estimates based on single laboratory data.

1.5 The DQCALC Software consists of a Microsoft Excel[3] workbook spreadsheet and associated macros and a user manual in Microsoft Word.[3]

2. Referenced Documents

2.1 *ASTM Standards:*[4]

D2777 Practice for Determination of Precision and Bias of Applicable Test Methods of Committee D19 on Water

D6091 Practice for 99 %/95 % Interlaboratory Detection Estimate (IDE) for Analytical Methods with Negligible Calibration Error

D6512 Practice for Interlaboratory Quantitation Estimate

2.2 *ASTM Adjuncts:*

DQCALC Microsoft Excel-based software for the Interlaboratory Quantitation Estimate (IQE)[2]

3. Terminology

3.1 *Definitions of Terms Specific to This Standard:*

3.1.1 *batch*—the samples associated with a given sample preparation. If all laboratories analyze samples prepared at three different times then results from each sample preparation would be considered a distinct batch.

3.1.2 *p-value*—probability value associated with curvature, the smaller the value the higher the likelihood of curvature (<0.05 is acceptable).

3.1.3 *Q-value*—Q must be positive and the associated probability of Q (p_Q-value) which is related to curvature must be <0.05.

3.2 *Acronyms:*

3.2.1 *DE*—detection estimate

3.2.2 *IDE*—interlaboratory detection estimate

3.2.3 *ILSD*—[inter or intra/within] laboratory standard deviation

3.2.4 *IQE*—interlaboratory quantitation estimate

3.2.5 *QE*—quantitation estimate

3.2.6 *SSR*—sum-of-squared residuals

[1] This practice is under the jurisdiction of ASTM Committee D19 on Water and is the direct responsibility of Subcommittee D19.02 on Quality Systems, Specification, and Statistics.

Current edition approved Dec. 15, 2016. Published December 2016. Originally approved in 2010. Last previous edition approved in 2010 as D7510 – 10. DOI: 10.1520/D7510-10R16E01.

[2] DQCALC is available from ASTM International Headquarters. Order Adjunct No. ADJDQCALC. Original adjunct produced in 2007.

[3] Trademark of Microsoft, Redmond, WA, 98052.

[4] For referenced ASTM standards, visit the ASTM website, www.astm.org, or contact ASTM Customer Service at service@astm.org. For *Annual Book of ASTM Standards* volume information, refer to the standard's Document Summary page on the ASTM website.

3.2.7 *WDE*—within-lab detection estimate

3.2.8 *WQE*—within-lab quantitation estimate

4. Minimum Requirements

4.1 DQCALC is based on an Microsoft Excel[3] spreadsheet workbook.

4.2 DQCALC requires the following minimum hardware and operating system configuration to function properly:

4.2.1 IBM-compatible PC with a Pentium microprocessor (or equivalent), 133 Mhz or faster.

4.2.2 Windows 2000 or XP.

4.2.3 Excel 2000, 2002 (XP), 2003, 2010, or 2013. Currently, DQCALC does not work with Microsoft Excel[3] 2008 or 2016.

4.2.4 32 MB RAM, plus minimum of 2–3 MB free disk space for each file to be processed.

4.2.5 Color video monitor, using a standard 1024×768 screen resolution. The program will function properly under any resolution, but may look awkward with other screen resolutions.

4.2.6 Mouse.

4.3 This application contains macros. You must have macros enabled in order for the program to function.

5. Basic Operation of DQCALC Software

5.1 *The Input File:*

5.1.1 The input file must be in the form of a Microsoft Excel[3] spreadsheet (see "example_input_file.xls"). Row 1 of the spreadsheet must contain the following column headers:

	A	B	C	D
1	Conc.	Result	Lab	Batch

NOTE 2—IMPORTANT: Any deviation from these headers will result in the input file being rejected.

5.1.2 There must be at least 5 unique spike-concentration levels with at least three instances of each concentration remaining after data preparation. The text format for all samples of the same concentration must be entered identically (for example, "5", "5." and "5.0" are considered different concentrations when checking for unique spike concentration levels).

5.1.3 A maximum of 1000 total records/result points are allowed.

5.1.4 Numbers that are stored as text in the input file will be handled, but any other text will be cleared and discarded.

5.1.5 Data sets with no concentration values (for example, true values) are allowed, but will be deleted in the Data Preparation process. Zero "0" is a valid value, but records containing text such as "blank" will be deleted.

5.1.6 Data sets with no value in the result column are allowed, but are discarded in DE & QE calculations. Entering "ND", "Not Detected", or any other Text string in the result column has the same effect of entering "0".

5.1.7 Both Lab and Batch columns must be filled in completely and they must be numeric. If there is only one batch or lab, enter the same number in all of the cells in that column (for example, "1").

5.2 *Operational Steps:*

5.2.1 Importing the data set file.

5.2.2 Conducting outlier removal, as appropriate.

5.2.3 Graphically evaluating the goodness of fit of the various models.

5.2.4 Selecting the appropriate model and calculating the detection estimate and quantitation estimates.

6. Obtaining the DQCALC Software

6.1 This software can be obtained by contacting ASTM (either by telephone or through the ASTM website) and requesting the DQCALC software.

7. Keywords

7.1 detection; DQCALC; IDE; IQE; quantitation