BETTER DATA LEADS TO BETTER DECISIONS

WLTR — SAAS DESIGNED FOR ANALYTICAL SCIENTISTS TO SELECT AND EVALUATE INITIAL CALIBRATION MODELS FOR OPTIMAL DATA DECISIONS

Written by the **WLTR Team**
REV_210706

INTRODUCTION

A laboratory relies heavily on analytical test equipment as a key component to help ensure the quality of reported data. The problem is human error. If your analytical bench chemists fail to make the proper initial calibration decisions your data quality suffers. The production of high- end quality data is a common goal shared by all analytical laboratories. However, one of the greatest short comings of analytical laboratories is the consistent production of high-end quality analytical data.

In principle, laboratories seek to build quality systems to produce high-end quality analytical data by minimizing random and systematic errors. Most established initial calibration acceptance criteria are established as a minimum pass/fail criteria; therefore, not all calibrations are created equal. If a laboratory could consistently achieve higher quality calibrations, the quality of the reported data is equally improved upon. Higher quality data then drives data confidence while improving the laboratory-client relationships resulting in higher corporate profits while minimizing liability exposure. **Better data leads to better decision!**

The source of that confidence is the specified accuracy of each instrument, and the foundation of that accuracy is the initial calibration. **Ultimately, the bedrock beneath the foundation of all analytical laboratories is the decisions made during the calibration of laboratory instruments.**

INSTRUMENT TRENDS

The evolution of analytical instruments and their associated data software program designs are in-large-part being driven by regulatory agencies requiring lower reporting limits while also achieving better accuracy and precision. Instrument manufacturers are responding with advances in instrument technology that can produce those data quality requirements which drives laboratories to purchase and/or replace aging instruments.

Instrument manufacturers are focusing their engineering efforts in the areas of producing user-friendly data handling solutions that are combined with smart instruments while miniaturizing the bench footprint. This approach, incorporating artificial intelligence, is designed to help improve preventive maintenance, lower the cost of ownership, and simplify the workflow, i.e., designing a turnkey solution for analytical laboratories.

Analytical instrument design engineers are focusing their efforts on functions such as automatic leak checks and troubleshooting diagnostics, which allow operators to achieve better and faster results with fewer mistakes. These innovative software and hardware instrument improvements are specifically designed to pro-actively guide users through preventative maintenance steps to help reduce unplanned downtime and sample reruns, greatly improving productivity.

Yet, as the manufacturing industry has evolved with changing technology, an added burden has also been placed on the analytical chemist and laboratory management to ensure they can meet these more stringent method and regulatory requirements. Innovations to instrument data acquisition and quantitation software has taken a back seat to design changes to the primary instrument and has not kept pace with the changing market demands. While instrument software has advanced to handle hardware design changes, it has not kept pace with an innovative software upgrade to validate the initial calibration data.

CHALLENGE: SELECTING INITIAL CALIBRATION VARIABLES USING ON- BOARDED INSTRUMENT DATA ACQUISITION SOFTWARE

BACKGROUND PROSPECTIVE

Historically, calibration models were typically selected using either an average response factor or a liner calibration model when building an initial calibration, where the instrument response is directly proportional to the concentration of the target analyte. These types of calibration models have some advantages, among them, simplicity and ease of use. However, as regulatory requirements have become more stringent, instrument technology has also had to evolve to keep pace with those requirements., (i.e., increase sensitivity and selectivity, linear dynamic range, etc.) With the evolving regulations and technology, analysts are increasingly likely to encounter situations where a linear model neither applies nor is appropriate, making calibration decision much more difficult for the bench analyst.

CALIBRATION MODEL SOFTWARE CHOICES

Most major manufacturers of gas chromatography (GC), liquid chromatography (LC) or ion chromatography (IC) instruments which produce chromatographic data have designed their software to allow the use of nine (9) distinct calibration models for data quantitation. These calibration models are as follows:

- Average Response Factor (A),
- Least Squared Equal Weighting (LS),
- Least Squared Inverse Concentration Weighting (LSIC),
- Least Squared Inverse Squared Concentration Weighting (LSISC),
- Least Squared Forced Zero (LSF0),
- Quadratic Equal Weighting (Q),
- Quadratic Inverse Concentration Weighting (QIC),

- Quadratic Inverse Square Concentration Weighting (QISC), and
- Quadratic Forced Zero (QF0).

Secondly with a plethora of instrument manufactures they also produce final data in various digital formats such as:

- text files,
- excel files,
- CSV files, or
- other comma delineated files etc.

Question (1): *With a large variety of instrument manufacturers and final data formats, is it possible to find a program that could capture this variety of calibration data into a single software program to check mathematical calibration models?*

Model considerations:

a) It is important to note not all mathematical models are allowed by regulatory bodies and /or auditing agencies,
b) some instrument manufacturers have designed their software to allow only certain calibration models, thus limiting the initial calibration choices analyst have when quantitating sample data,
c) there is no common naming scheme between manufacturers, which may cause major consternation for data users.

In fact, without an industry wide naming scheme, there have been instrument software revisions that have completely misnamed the mathematical models, where an analyst may be thinking they have chosen one model and in truth it may have been a completely different calibration model.

Question (2): *How can the analyst verify the calibration model chosen from the selection of on-boarded calibration models is the actual named calibration model chosen?*

Question (3): *How can the analyst verify and validate the mathematical calibration models chosen from the selection of on-boarded calibration models are mathematically correct?*

INITIAL CALIBRATION CONSTRUCTION VARIABLES

Calibration of analytical instruments producing chromatographic, spectrophotometric or other similar types of data, generally require delineating or modeling the relationship between the response of the instrument and the concentration or mass of an analyte introduced into the instrument. Most instrument software will produce a graphical depiction of this relationship and is often referred to as the calibration curve.

When building a new analytical method, the type of calibration must be considered, as it plays a critical role in data quantitation. There are two major types of instrument calibration, that are used in the quantitative analysis of chromatographic data:

a) external standard calibration, and
b) internal standard calibration.

The analyst that constructs a calibration curve must navigate several key decision points in the evaluation and final choice of the mathematical model chosen for calibration. Each mathematical model has evaluation parameters that need to be reviewed to assess precision and accuracy such as relative standard deviation (RSD), correlation coefficient (r) or coefficient of determination (r^2). These evaluation parameters or mathematical functions also have evaluation criteria specified for each evaluation parameter which establishes a minimum pass/fail threshold to use a particular calibration model.

Question (4): *How can the analyst, construct, review, select and evaluate a calibration model when relative standard error (RSE), percent error (PE%), minimum RF, etc. are not calculated by the on-boarded CDS instrument software?*

Question (5): *The analyst generally re-quantitates the initial calibration standards against itself to determine the calibration metrics for the purpose of making final model decisions. This process is riddled with potential mistakes and is extraordinarily inefficient. How can the analyst ensure calibration model evaluations can be evaluated, verified and validated?*

CALIBRATION STANDARDS

Initial calibration for chromatographic methods involves the analysis of standards containing target analytes at varying concentrations defining the working or calibration range of the instrument. Sample are then analyzed on the instrument that was configured to identify those target analytes and to produce concentration values based on the chosen mathematical calibration model.

Question (6): *How can the analyst verify initial calibration standards have been correctly prepared and ensure the construction of the calibration does not contain a rogue standard(s)?*

NUMBER OF CALIBRATION POINTS AND CONCENTRATION VALUES

Standards are generally prepared by serial dilution of a stock standard and will form a geometric series of concentration points where each standard will vary from adjacent standards by a constant factor. However, this may produce relatively wide spacing of the higher concentration standards in the geometric series masking the situation where the detector is reaching saturation. Analytical procedures which contain a large analyte list may have target analytes that are at saturation and need to be dropped from the initial calibration while retaining those same concentration points for other target analytes.

Question (7): *How can the analyst understand analyte saturation as well as calibration concentration spacing?*

Most regulatory agencies specify the minimum number of calibration standards for average response factor or linear (first order) calibration models and for quadratic (second order calibration models).

Question (8): *How can the analyst ensure the minimum number of calibration standards have meet the method criteria for each target analyte?*

CALIBRATION RANGE AND REPORTING LIMIT

Once the calibration points have been chosen, the concentration points within the initial calibration define the working range of the instrument where the highest-level calibration standard establishes the upper level of quantitation.

The lowest calibration standard that is analyzed during the initial calibration generally must be at or below the established reporting limit and is considered the Lowest Level of Quantitation (LLOQ) or Reporting Limit (RL). The concentration of this standard is related back to sample concentration using sample size, dilution, and final volume. Therefore, the initial calibration must contain at least one standard at or below the calculated reporting limit. Currently, using on- boarded CDS instrument software, this is a manual evaluation and most likely is not being evaluated at all.

Question (9): *Most calibrations are constructed using concentration units such as ug/L (PPB) or ug/ml (PPM). Samples typically undergo some type of extraction or preparation prior to sample analysis where a multiplier is applied to the concentration units generated during the final report generation. Since there is typically a sample multiplier, how can the analyst ensure the lowest calibration standard included in the construction of the initial calibration is at or below the required reporting limit?*

EXTRAPOLATION AND ZERO (0) RESPONSE

Analysts generally prepare calibration standards that cover the concentration ranges appropriate for programs, projects or types of analyses. Extrapolation of the calibration to concentration values either above or below those of the actual calibration standards are generally not appropriate as they may lead to significant quantitative errors regardless of the calibration model chosen.

When calibration models are evaluated with current instrument software, users do not know if the LOQ/RL will generate a positive concentration value, (i.e., a positive y-intercept.) The only option open to users is to re-quantitate the initial calibration against itself. In addition, many laboratories are required to report data below their actual reporting limit and/or report down to their statistically derived method detection limit (MDL) as an estimated value.

Question 10): *How is an analyst able to prove data reported below their lowest calibration point is:*

a) at a concentration value that is above the y-intercept and will produce a positive value,
b) the calculated concentration follows the predicable monotonic mathematical model, and
c) a zero (0) response does not produce a calculated concentration that is above the LOQ/RL?

CURVE REFITTING

Many regulatory programs require laboratories to review their initial calibration curve for bias by performing a curve refitting inspection. This is generally not an alternative to evaluating the initial calibration mathematical model selection, using the historically accepted practice, i.e., RSD, correlation coefficient (r) or coefficient of determination (r^2), but is used in conjunction with those calibration parameters to help inspect and evaluate the calibration curve. There are two general approaches to inspect the calibration curve, and both curve refitting procedures evaluate the difference between the measured amount and the true amounts used to create that model. These two procedures are the calculation of percent error (PE%) or bias and relative standard error (RSE)

Question (11): *How can the analyst ensure the initial calibration has been reviewed and verified for curve refitting criteria?*

SOLUTION: SELECTING INITIAL CALIBRATION VARIABLES USING WLTR AS YOUR PERSONAL DATA ASSISTANT

WLTR — BETTER DATA DECISION

The following discussion dissects current CDS software limitations by answering the questions posed above and describes the features built into WLTR to solve those problems.

WLTR - SOFTWARE AS A SERVICE (SAAS)

Current laboratory instrument CDS software servers a utilitarian purpose and is generally grounded in good software engineering and proven calibration mathematics. However, most chromatography software designs employ a myopic data visualization approach and software engineers have failed to update the architectural design structure of this software in keeping pace with advancing and changing instrument technology. The data produced by on-boarded instrument CDS software is presented in a format that is clumsy, inefficient, is not well organized, and does not include all the calibration metrics most laboratories are seeking; therefore, it needs a visionary new look. In general, there are few arguments regarding calibration model mathematics; however, there are issues that should be addressed regarding three (3) key functional areas:

1. better data visualization
2. understand how to process initial calibration data, i.e., “raw” data acquired by on- boarded CDS software, and evaluate it in a manner allowing the analyst to make better informed calibration decision, and
3. understand how better calibration decisions will increase data quality.

WLTR was designed and developed to provide instrument users a mathematically based platform to compute, construct, display, review, select and evaluate initial calibrations using a novel data visualization

deck (DVD) summarized in the initial calibration summary table. This data-design structure was specifically engineered to help aid the bench chemist, make better calibration decisions, produce better quality data and provide the analyst a personal data assistant (PDA), i.e., an evaluation tool.

WLTR addresses these areas of weakness, and the result is:

- a more efficient analyst,
- better calibration decisions producing higher quality data,
- a data quality mechanism to document calibration metrics and increase profitability, and
- a fiduciary commitment by laboratory owners to minimize calibration errors and mathematically validate initial calibrations, hence an insurance policy.

WLTR incorporated numerous functions allowing the user to manipulate the initial calibration construction. These calibration variables and evaluation parameters are encapsulated in the initial calibration summary table enabling the user to make mathematically based calibration decisions.

SOFTWARE UPLOADS USING VARIOUS DIGITAL FORMATS

Question (1): *With a large variety of instrument manufacturers and final data formats, is it possible to find a program that could capture this variety of calibration data into a single software program and check mathematical calibration models?*

WLTR was designed to electronically read and digitally incorporate a large variety of data formats into a single program; in the same manner as a Laboratory Information Management System (LIMS) is designed.

WLTR can accommodate the following types of digital data formats:

- text files,
- excel files,

- CSV files, or
- other comma delineated files etc.

CALIBRATION MODEL NOMENCLATURE

Question (2): *How can the analyst verify the calibration model chosen from the selection of on-boarded calibration models is the actual named calibration model chosen?*

WLTR was written and coded to mathematically calculate the nine (9) most common calibration models used in chromatography software. Secondly, the acquired "raw" data used to construct or build an initial calibration is the same data uploaded into WLTR, so there is a direct digital data correlation. Thirdly, WLTR can accommodate up to twenty (20) calibration points; allowing data points to be deleted or manipulated in the same fashion as the on-boarded CDS instrument software.

The key to verifying and identifying the named calibration model is quantitating an independent sample, (i.e., the initial calibration verification (ICV) standard,) against the initial calibration. The ICV is a standard typically purchased from a source of standards independent of the source used to prepare the initial calibration standards and its purpose is to verify the initial calibration standards were properly prepared. This standard has an added benefit when uploaded into WLTR; it is used to independently compare the computational mathematics produced by both software programs, (i.e., it independently validates the calibration mathematics.)

Once digital data is uploaded, WLTR computes, constructs and displays all calibration points for all nine (9) mathematical models. It also computes all initial calibration points quantitated against the constructed mathematical model and displays the data for all data points up to a maximum of twenty (20) data points. On-boarded CDS software is not capable of these computations in real-time, nor can they display all possible calibration models, or display all calibration points!

Finally, WLTR computes the ICV target analytes against the constructed initial calibration using the chosen calibration variables and displays the data quantitated against all nine (9) mathematical models. The ICV target analyte value(s) quantitated by the on-boarded CDS software is also displayed; therefore, the data set that has matching concentration values verifies the named mathematical model.

VALIDATING CALIBRATION MATHEMATICS

Question (3): *How can the analyst verify and validate the mathematical calibration models chosen from the selection of on-boarded calibration models are mathematically correct?*

WLTR independently computes all calibration models from the "raw" uploaded data. WLTR is used to evaluate all possible calibration variables that are then used by the analyst to modify the on-boarded instrument software to construct the instrument calibration. The analyst then re-quantitates the initial calibration verification (ICV) standard using the on-boarded revised method and uploads the newly re-quantitated ICV into WLTR.

WLTR computes the concentration values for the ICV target analytes against all possible mathematical calibration models and displays the concentration values determined by WLTR as well as the concentration values determined by the on-boarded instrument software.

WLTR uses the Data Visualization Deck (DVD) to display both sets of data and calculates the percent error (PE%) between the two values. The re-quantitated concentration values from the instrument on-boarded CDS software will now produce the same calculated concentration values, within the errors produced by rounding, for each target analyte as calculated by WLTR for the selected calibration model.

WLTR uses a proprietary process to validate the initial calibration using three metrics:

1) it verifies the initial calibration variables used in the WLTR program are also the same calibration variables selected for the on-boarded

instrument software,

2) it verifies and validates the chosen mathematical model, and

3) it verifies and validates the mathematical functions and naming scheme.

INITIAL CALIBRATION CONSTRUCTION VARIABLES

—

Question (4): *How can the analyst, construct, review, select and evaluate a calibration model when RSE, (PE%), minimum RF parameters are not calculated by the on-boarded instrument software?*

As previously discussed, the instrument manufacturing side has evolved significantly in the past several decades; incorporating artificial intelligence to help improve preventive maintenance, lower the cost of ownership, and simplify the workflow, (i.e., designing a turnkey solution for analytical laboratories.) However, instrument software has not kept pace with the changing market demands, and manufacturers have not focused their software design efforts that would make a true QA/QC turnkey solution for analytical laboratories!

WLTR was designed as a SaaS program that can evaluate both internal or external calibrations using uploaded “raw” data in a variety of digital or electronic formats.

WLTR was NOT designed as a concept or as a replacement to on-boarded CDS instrument software but was conceived and designed as a true working program; used in my laboratories for approximately twenty (20) years. The need for such a software program to compute, construct, display, review, select and evaluate calibration data has never had a greater demand for its use than today!

WLTR has incorporated five (5) novel software design features that will empower the user to quickly assimilate data allowing unprecedented calibration decisions.

1. A unique platform to review the initial calibration described as a Data Visualization Deck (DVD).
2. The ability to change calibration variables, in real-time, allowing the

user to visualize how those changes affect the re-quantitation of each initial calibration point for all mathematical model options.

3. A software feature that incorporates calibration evaluation parameters not currently programed into on-boarded instrument software, i.e., %RSE, PE%, SPCC, CCC etc.
4. A software feature that allows the user to input initial calibration criteria for each calibration evaluation parameter.
5. A software feature that performs an overall evaluation of the initial calibration for all evaluation parameters using the evaluation criteria input by the user.

The result is a personal data assistant (PDA), leading to better decision-making and optimal data quality.

INITIAL CALIBRATION – RE-QUANTITATE DATA IN REAL-TIME WITHOUT MANUAL RE-QUANTITATION

Question (5): *How can the analyst ensure calibration models are being properly reviewed, verified and validated before they are put into production?*

With on-boarded instrument software, the analyst must first collect the initial calibration data and start the process of calibration construction. This involves making construction decisions, viewing one analyte at a time and scrolling through additional windows to see a calibration plot, RSD and correlation coefficient or r values. After the first rough calibration decisions are made, the analyst re-quantitates the standards against itself to get a second look at the calibration. This is generally required to help the analyst understand the calibration metrics in making final model decisions. This process is riddled with potential mistakes and is extraordinarily inefficient. In addition, many laboratories do not re-quantitate their initial calibration against itself; they simply choose calibration parameters and proceed with data analysis without understanding curve refitting functions etc.

WLTR, with the five (5) major software design features, allows the user to construct the initial calibration and/or modify the initial calibration and

understand real-time how the calibration metrics change with each calibration decision point change. The RF, RSD and a host of many more calibration parameters are calculated and displayed in the data visualization deck (DVD) for each target analyte.

As an example, if the RSD, for a target analyte is above an established acceptance criteria, the analyst may decide the RF value of one or more calibration points is producing the high RSD. WLTR will allow the analyst to easily eliminate any single calibration point or a combination of calibration points anywhere in the calibration. Each time a change is made the remaining calibration points are automatically re-quantitated in real-time for all nine (9) mathematical models as well as updating all the calibration parameters.

The analyst will know immediately, how changes to the construction of the calibration will affect the overall evaluation of the initial calibration. This process performed using the on- boarded instrument software is tedious, time consuming, riddled with possible mistakes, and inefficient.

WLTR is extraordinarily efficient, as it will evaluate, verify and validate the initial calibration in real-time, saving an enormous amount of time, and eliminating all possible evaluation mistakes while validating the calibration against the evaluation parameters.

CALIBRATION STANDARDS

Question (6): *How can the analyst verify the initial calibration standards have been correctly prepared and ensure the construction of the calibration does not contain a rogue standard(s)?*

WLTR was designed with a multitude of unique software features allowing the user to efficiently conduct an initial calibration review, facilitating the search for suspected mis-made or rouge standards. There are two approaches the user could employ for this type of evaluation as follows:

1) WLTR has a built-in data visualization deck (DVD) allowing, the user, unfettered viewing of the initial calibration construction. This

includes the graphical depiction of five of the nine plotted calibration curves for each target analyte. By scrolling through each target analyte and viewing these graphs, mis-made, or rogue standards should be apparent to the data viewer. There are no numeric metrics associated with this quick visualization scan other than:

A picture paints a thousand words

2) WLTR will display the calculated concentration values for each target analyte included in the initial calibration verification (ICV) standard loaded into the software. The user selects the true concentration values of this standard the same as for the true concentration values of the initial calibration points. WLTR will evaluate the ICV against the criteria the user chooses, and a rogue standard could be found by reviewing the ICV for percent difference against the know true value, (i.e., a bias evaluation.) WLTR will perform this evaluation instantaneously and will summarize and document the data in the initial calibration summary table.

TARGET ANALYTE SATURATION AND INITIAL CALIBRATION POINT SPACING

Question (7): *How can the analyst understand analyte saturation as well as calibration concentration spacing?*

WLTR displays the calibration plots along with the RF values allowing the analyst to see the direct correlation between these two items in the data visualization deck. The visualization of the calibration plots directly associated with the RF values for each calibration point gives great data insight into both concentration spacing as well as analyte saturation.

EVALUATING THE MINIMUM NUMBER OF CALIBRATION POINT

Question (8): *How can the analyst ensure the minimum number of calibration standards have meet the method criteria for each target analyte?*

This is such an easy task one may wonder, why is this important. It becomes important when an analyst is calibrating a method with a large target analyte list where these minor calibration issues are easily overlooked.

One of the five novel software design features incorporated into WLTR is a feature allowing the user to input, review, verify and validate calibration parameters not currently programed into on- boarded instrument CDS software. The user can input the minimum number of calibration points needed to use for:

- an average RF calibration model,
- a linear regression calibration model, or
- a quadratic regression calibration model.

WLTR will evaluate each target analyte, determine the mathematical model chosen, and count the number of calibration points the analyst chose for that calibration model. WLTR will then display its findings in the initial calibration evaluation table indicating if that set of calibration parameters met the criteria to allow its' intended use.

EVALUATING THE INITIAL CALIBRATION FOR REPORTING LIMIT

Question (9): *Most initial calibrations are constructed using concentration units such as ug/L (PPB) or ug/ml (PPM). Samples typically undergo some type of extraction or preparation prior to sample analysis where a multiplier is applied to the concentration units during the final report generation. Since there is typically a sample multiplier, how can the analyst ensure the lowest calibration standard included in the construction of the initial calibration is at or below the required reporting limit?*

WLTR allows the user to input, review, verify and validate calibration parameters not currently programed into on-boarded instrument software. The user can input the laboratory required reporting limit (LOQ/RL) for each target analyte for two separate matrices such as soil

or water. The units used for the initial calibration are mathematically transformed into the reporting units established for the final report using the multipliers for each matrix input by the user.

WLTR will evaluate and display those findings in the initial calibration evaluation table indicating if the lowest calibration point chosen for a particular target analyte met the minimum reporting limit goal.

EXTRAPOLATION AND ZERO (0) RESPONSE

Question (10): *How is the analyst able to prove data reported below the lowest calibration point is:*

> ***a)*** *at a concentration value that is above the y-intercept and will produce a positive value,*
> ***b)*** *the calculated concentration follows the predicable monotonic mathematical model, and*
> ***c)*** *a zero (0) response does not produce a calculated concentration that is above the LOQ/RL?*

WLTR, through the data visualization deck, allows the user to quickly assimilate data and review the re-quantitated or recalculated concentration value of each initial calibration point for all mathematical model options ensuring concentration values below the reporting limit will produce positive values.

WLTR uses the lowest chosen calibration point and estimates concentration values below the lowest limit of quantitation standard at 0.75%, 0.50%, 0.25%, 0.125% and zero response for all nine (9) calibration models by extrapolating the mathematical model residuals. Therefore, the estimated concentration values below the LOQ/RL can be proven to follow the monotonic mathematical model.

WLTR estimates the zero (0) response concentration for each mathematical model and displays that information on the DVD. In addition, the linear dynamic range (LDR) study for the chosen mathematical model for each analyte is summarized in the summary report and includes the estimated concentration for the zero (0) response.

CURVE REFITTING

Question (11): *How can the analyst ensure the initial calibration has been reviewed and verified for curve refitting criteria?*

WLTR, calculates both RSE and PE% evaluation parameters which are the two curve refitting functions generally used to review and verify curve refitting criteria. As the user constructs the initial calibration, they see these calibration metrics change real time with each calibration decision point change. As discussed earlier, the software incorporates calibration evaluation parameters not currently programed into on-boarded instrument software such as RSE, PE%, etc.

WLTR allows the user to input initial calibration criteria for each calibration evaluation parameter including RSE and PE%. These values are calculated and displayed on the data visualization deck (DVD) as well as the initial calibration summary table.

WLTR calculates PE% bias results for each calibration point for all mathematical models for each target analyte. Initial calibration points having a calculated bias greater than the value chosen by the user will be flagged.

WLTR also evaluates the RSE value for the chosen mathematical model and displays that information on the data visualization deck and in the initial calibration summary table.

WLTR electronically extracts the PE% bias results and displays that data in the Linear Dynamic Range (LDR) Study report for each target analyte.

IDENTIFYING INITIAL CALIBRATION DATA ISSUES AND FINAL DOCUMENTATION

WLTR incorporates novel architectural software design features which allow the user to quickly compute, construct, display, review, select and evaluate initial calibration model selection.

WLTR independently calculates the initial calibration mathematical models for each target analyte using the “raw” data uploaded into the SaaS program. This program will produce true independent validation of the initial calibration.

WLTR summarizes the initial calibration using the method evaluation parameters and the user selected evaluation criteria in the initial calibration evaluation table. This allows the user to identify initial calibration data issues as well as final documentation of the initial calibration.

A METADATA APPROACH TO CONSTRUCT BEST-FIT INITIAL CALIBRATION MODELS ACHIEVING BETTER DECISION OUTCOMES

WLTR, as a mathematically based SaaS program, will independently compute, construct and display the initial calibration for each target analyte. This program then uses logic functions to review the selected calibration variables against evaluation parameters.

WLTR takes a metadata approach using logic functions to evaluate, validate and document all major and minor construction variables chosen by the user for each target analyte.

WLTR is a user-friendly tool performing all the calculations independent of the on-boarded CDS software and displays that information on a data visualization deck (DVD) that is truly unique.

WLTR is the answer to questions regarding software limitations users encounter with on-boarded instrument CDS software.

DRIVING PROFITABILITY

This industry needs a solution to review, verify and validate the initial calibration, produced from the instrument on-boarded CDS software, using a program that independently calculates the calibration parameters and evaluates the initial calibration against chosen calibration criteria.

WLTR which incorporated the five novel software design features drives financial profit metrics as follows:

- analysts can make initial calibrations construction decisions exponentially faster,
- calibration issues or problems will be flagged by the software enabling the analyst to reevaluate those initial decisions eliminating calibration construction mistakes,
- better fit initial calibrations will produce better data quality,
- better quality data lowers the laboratories exposure to liability issues, and that
- translates to higher corporate profits!