



SITE SPECIFIC TEST METHOD GUIDELINE

Fuels Analysis and Methods Evaluation Section
Chemical Analysis and Emissions Research Branch
Mobile Source Laboratory Division

DISCLAIMER: This procedure has been reviewed by the staff of the California Air Resources Board and approved for publication. Mention of any trade name or commercial product in this Standard Operating Procedure does not constitute endorsement or recommendation of this product by Air Resources Board. Specific brand names and instrument descriptions listed in the Standard Operating Procedure are for equipment used by the Air Resources Board laboratory.

AIR RESOURCES BOARD GUIDELINES FOR PETITIONS FOR SITE-SPECIFIC ALTERNATIVE TEST METHODS FOR CBG FUEL PROPERTIES

These guidelines summarize the requirements that the Air Resources Board (ARB) believes site-specific alternative test methods should satisfy and the information that should be included in petitions for approval of site-specific alternative test methods. Approval of a site-specific alternative test method by the ARB means the ARB declares that method equivalent to an ARB designated test method. Guidelines for informing the ARB of major changes to previously approved alternative test methods are also included in this document.

A site-specific test method is a test method whose performance has been validated for a particular refinery or group of refineries owned by a single company for the product streams of these refineries. (For brevity, a location where the method is to be used will often be referred to as a refinery or a site). Site-specific methods may be on-line measurement methods integrated into an on-line blending system, or they may be methods that are used off-line, but have been validated only for a specific refinery or group of refineries.

A company interested in having the ARB declare its site-specific test method equivalent to a designated method should begin the process by submitting a petition to the ARB's Executive Officer. The ARB staff will review the analytical technique, the relationship between designated and proposed alternative methods, and the quality assurance and quality control (QA/QC) procedures (protocol) to determine if the proposed method provides results that are equivalent to results produced by the designated test method. If the proposed method is found to provide equivalent results, an Executive Order will be issued which finds the site-specific method equivalent and describes the conditions under which it can be used. The Executive Order may also identify the circumstances under which it would be rescinded.

The ARB recommends that a draft petition be submitted to the ARB staff for preliminary review prior to submission of a formal petition to the ARB's Executive Officer. This preliminary review is for the purpose of determining the completeness of the submission and providing ARB and industry technical staff an opportunity to informally discuss the candidate test method and the ARB's technical review process.

The petition for equivalence should contain the following six elements:

1. A petition letter to ARB's Executive Officer
2. A description of the on-line blending technique (if applicable)
3. Documentation of the proposed method
4. An in-depth evaluation of the relationship between the proposed and the ARB-designated method

5. The QA/QC protocol to be applied during the operation of the method
6. A statement affirming that the statistical calculations described in Appendix B have been carried out using a spreadsheet that performs the calculations in the appendix, the spreadsheet having been found by one of the statisticians designated by ARB to be in accord with the appendix

These elements are described in more detail in paragraphs I-V of this document. Paragraph VI describes guidelines for informing the ARB of major changes to previously approved alternative test methods.

I. THE PETITION LETTER

The letter should be addressed to the ARB's Executive Officer, with a copy sent to the Chief of the Monitoring and Laboratory Division. The alternative test method should be given a name that completely identifies it, including the company, site(s), type of measurement, and fuel property being measured.

The letter should explain whether the method will be used on-line or in batch mode. If the method is not used on-line and is not an empirical method derived specifically for the specific site(s), the petition should explain why the method cannot be subjected to interlaboratory testing. The letter should also provide the name of a contact person who is familiar with the method and the relevant quality control procedures. The telephone number, fax number, and e-mail address (if applicable) of the contact person should be provided.

II. THE ON-LINE BLENDING TECHNIQUE (IF APPLICABLE)

Include a diagram and description of the on-line blending technique if the alternative method analyzer is integrated into an automated blending system. This section of the petition should explain how the on-line analyzer is integrated into the blending system and how on-line analyzer values are combined to produce a final gasoline property value for the blend. A sample calculation of final property values from on-line analyzer measurements should be included.

III. DOCUMENTATION OF THE PROPOSED METHOD

A specification of the proposed method, written in the style and format of a Standard Test Method of the American Society of Testing and Materials (ASTM), should, at a minimum, contain all of the following elements:

1. **Scope Statement** - The scope statement should define the concentration (or property) range to which the method will be applied. This is the range in which the method has been validated and within which adequate precision can be obtained. The relevant fuel parameters of the gasolines that are to be measured by the method must be characterized in sufficient detail. The parameters of the gasolines historically produced by the refinery units to which the method will be applied should be identified.
2. **Limitations** - Known interferences, matrix effects, and other limitations of the method should be described in this section. Discuss how these

- interferences and matrix effects are accounted for, either by the method itself or by the statistical modeling.
3. **Summary of Test Method** - The detection principle of the method should be described along with the process by which raw data are transformed to obtain a final result.
 4. **Referenced Documents** - References to standard practices or procedures that are incorporated in the test method.
 5. **Apparatus** - A description of the instrument and accessories used for the analysis.
 6. **Procedure** - Summary of the steps taken in routine operation of the method.
 7. **Calculations** - The calculation of the final reported alternative method result for a tank should be described in detail. For on-line analyzers, the averaging of multiple measurements to obtain predicted tank final or composite final values should be described.
 8. **Calibration** - A description of the calibration data, procedures and results should be included in the petition. In some cases but not necessarily all, calibration would include establishment of a relationship between site-specific alternative test method values of a fuel property and corresponding designated test method values.
 9. **Validation** - Validation is the verification that the calibration process was such that alternative test method results are adequate predictors of designated test method results. Validation is done with a representative set of gasolines that was not used in the calibration process. Section IV and Appendix A contain a detailed description of the information about validation that should be included in the petition.
 10. **Quality Assurance and Quality Control** - The protocols for quality assurance and quality control should be stated in detail, including statements of the quantitative statistical properties of the quality control protocol. Section V contains a more detailed statement of these requirements.

IV. INVESTIGATION OF THE RELATIONSHIP BETWEEN THE ALTERNATIVE AND DESIGNATED METHOD RESULTS

Designated method values predicted by an equivalent alternative method will have the same status in fuel property regulations and calculations as designated method values have. Equivalence of an alternative method implies that use of this method and the designated method should have the same consequences. The investigation of the relationship between designated test method results and alternative test method results (described in Appendix A) provides evidence of whether or not this criterion is plausibly satisfied.

In most cases, the relationship between the designated test method values and the alternative test method values will be investigated using statistical methods including linear regression. Regression is a means of establishing a relationship

between the two sets of values. The analysis must also quantify the residual variation about the regression line in order to quantify the uncertainty of predicted designated method values. The uncertainty, which may be property-dependent, may not exceed a certain limit. If the uncertainty exceeds this limit for some range of fuel property values or some fuels, the alternative method may not be used for these values or fuels. Computation of the uncertainty and comparison with the limit is discussed in detail in Appendix A.

Appendix A gives a more technical general description of the statistical regression modeling that is usually performed and describes the documentation of the data and the modeling results that should be included in the petition.

V. QUALITY ASSURANCE AND QUALITY CONTROL

The protocol must include provisions for quality assurance that will ensure that the alternative method continues to meet the goal of performance equivalent to that of the designated method. Regular crosschecks between the alternative and designated methods must be performed to ensure that the statistical relationship between the alternative and designated methods remains stable. The quality assurance (QA) protocol must state explicitly the frequency of parallel testing between the designated and alternative methods that will take place after the method has been approved. Plotting the results on control charts is essential. The use of special types of control charts such as cumulative sum (cusum) charts that are especially sensitive to systematic bias should be considered. If different "families" of gasolines are measured by the alternative method, cross checks should be performed regularly for all the families.

In cases where a QC program is used to measure the long-term stability of the alternative test method, the petition for method equivalency should include a QC protocol that states performance goals, describes all checks performed, and describes computations by which control limits are set. The statistical properties of the QC protocol, for example the average time required to detect shifts of the mean large enough to be of concern, should be discussed. A quality control (QC) program is not mandatory.

Changes in fuels or in the implementation of the alternative method may impact the long-term stability of the relationship between the two methods. Users of an alternative method should not rely only on control charts to detect significant changes in the relationship between designated and alternative method. They should also plan to anticipate potential changes in the relationship due to modifications to apparatus and operational procedures and changes in feedstocks, and perform intensive crosschecking at these times, to ensure that the existing relationship between the methods is not significantly affected by the changes.

The QA/QC protocol must provide specific answers to for the following questions:

1. What steps are taken when an out-of-control situation occurs?
2. What steps are taken to anticipate changes in blend stocks that can affect the performance of the analyzer?
3. What steps are taken when a modification to the test method takes place?
4. What steps are taken when crosscheck results show a significant difference in results between the designated and alternative methods?

ARB staff will provide input on QA/QC requirements during evaluation of the draft petition.

Samples to be used as QA or QC samples should be representative of the gasolines produced at the site. They need not be tank final or composite final samples.

Companies must monitor the performance of alternative test methods with QA samples. Companies may choose to use QC samples as an additional check.

VI. INFORMING THE ARB OF MAJOR CHANGES TO A PREVIOUSLY APPROVED ALTERNATIVE METHOD

Major changes to a previously approved alternative test method may be needed for several reasons: changes in instrumentation, changes in feedstocks, changes in the refining process, modifications of the blend formulas to be measured by the method, changes in the range of the fuel property, evidence that the model does not predict designated method values for some gasolines well enough, etc. Major changes are significant modifications of the details of the method that do not change the types of measurements being made and the type of relationship with the designated method. Changes in these would require a new petition. This document does not attempt a precise definition of a major change; anticipating all the special cases would be impossible.

An alternative test method is declared equivalent on the basis of a thorough understanding and documentation of its properties and its satisfactory performance. Refiners are expected to maintain detailed records documenting changes in conditions affecting the method and changes made to the method, whether major or not.

Because alternative fuel test methods, if used, play an essential role in ensuring that gasolines satisfy ARB fuel regulations, the refiner must inform the ARB that major changes are being made to an alternative method. The ARB may waive this requirement for individual methods, in whole or in part, after there is sufficient experience with routine operation of the method and making major modifications to the method.

Since the equivalent method is initially required to satisfy strict conditions, it is acceptable to document major changes in significantly less detail than the documentation of the original petition. The ARB may in some cases request more detailed documentation of major changes.

The ARB should be informed that a major change is being made to an equivalent alternative method by a letter to the Chief of the Monitoring and Laboratory Division. Like the original petition, the letter should summarize (but more briefly) the evidence supporting the refiner's conclusion that the modified alternative method will meet the equivalency requirements.

The letter should briefly document:

1. The reasons why the petitioner is making a major change to the method
2. The types of changes to be made to the method
3. The change, if any, in the scope of the method
4. If the alternative method is being revalidated, the revalidation data set
5. Changes in the set of gasolines (set of alternative method data) for which the limit on **acceptable** variability of predicted designated method values is not exceeded (see Appendix A)
6. Plans for more intensive QA/QC to verify that the modified method is initially performing satisfactorily
7. Any plans for updating the modified method after more comprehensive data relating it to the designated method are obtained

Data for revalidation of the relationship after a major change - Data sets for revalidating the relationship between alternative and designated method values after a major change are necessarily a compromise between the need for adequate representation and the desire to promptly begin using the revised method. The general guidelines for satisfactory validation data sets stated in Appendix A are equally applicable to data sets used for revalidation. A revalidation data set must be at least minimally representative of both the range of fuel property values and the gasolines for which the alternative method will be used.

APPENDIX A

TECHNICAL DETAILS OF VALIDATING THE RELATIONSHIP BETWEEN THE ALTERNATIVE AND DESIGNATED METHODS

Validation is the verification that the calibration process was such that alternative test method results are adequate predictors of designated test method results. Validation is mandatory and must be done with a representative set of gasolines that was not used in the calibration.

This appendix summarizes the properties of satisfactory data sets for validating the relationship between alternative and designated test method data, gives a general description of the type of statistical modeling that is usually performed, and states the "reproducibility" requirement that an alternative method must meet.

The petitioner's own needs for a dependable high-quality relationship between alternative and designated method measurements and these ARB guidelines together impose a number of requirements on the data and analyses that support the alternative method. The petitioner will have concluded, before submitting the petition to the ARB, that the alternative method reasonably satisfies these requirements. The purpose of the documentation suggested by these guidelines is to substantiate this conclusion in reasonable detail. Because validation is an essential step in establishing that an alternative method is equivalent, limiting the discussion of validation to the correspondence of the predicted designated method values to measured designated method values is far from sufficient.

The Validation Data Set - The petition for approval of the test method must show that the validation data set adequately represents the gasolines for which the modeled fuel property will be measured by the alternative method.

The validation data are paired alternative method and designated method results on gasolines produced in the refinery or made elsewhere from the refinery's blending components.

Values of the modeled fuel property should span its entire range over the gasolines for which the alternative method is to be used. There should not be gaps in the values of the fuel property so large that they raise doubts about whether the relationship is well determined in the gaps or on either side of them. If the values of a modeled property of gasolines produced by a refinery fall into two or more clusters separated by large gaps, fitting a separate model to each cluster of values should be considered.

Adequate representation of the relevant multi-dimensional set of values of other fuel properties that significantly affect the relationship is required, in addition to representation of values of the modeled fuel property. Representation of relevant extreme points in the multi-dimensional space of fuel parameters is especially important. Adequacy of representation cannot be guaranteed by mere numbers of data points. The amount of data needed to validate the relationship must necessarily be determined on a case-by-case basis.

Systematic inclusion in the data sets of gasolines produced using a site's blend formulas is an obvious first step towards adequately representing the values of relevant gasolines and fuel properties. Petitioners should consider whether current blend formulas adequately represent all of the gasolines that they will want to certify by the alternative method.

Measurements of hand blends and measurements of samples taken at intermediate stages of blending a tank, and tank final and composite final samples may all be included in validation data sets. However, the inclusion of tank final or composite final samples is not required.

The calibration and validation data sets must be made available to the ARB in machine-readable form upon request.

Statistical Regression Analysis - A relationship between designated method values and alternative method data will usually be derived by a standard linear regression analysis. The regression must be shown to have statistical properties that make a convincing case for equivalence. Establishing the relationship will often require multiple iterative improvements. The petition may describe and evaluate only the final relationship; intermediate validation steps need not be described.

The recommended, standard regression models and the associated methods for estimating the uncertainty in designated method values predicted from alternative method values are described in Appendix B. The models are commonly used in applied statistics even though they depend upon assumptions that may not be very well satisfied. The recommended regression methods are based on the following assumptions:

1. there are no errors in the values of the independent variable (the alternative method data)
2. the errors in the values of the dependent variable (the designated method data) are normally distributed
3. the variance of the errors in the values of the dependent variable is constant over the range of values of the independent variable

Definitions:

$\{Y_i : i = 1, \dots, n\}$: Designated test method results (values) on the validation samples. Y is the dependent variable in the regression analysis.

$\{X_i : i = 1, \dots, n\}$: Alternative test method results (values) on the validation samples. X is the independent variable in the regression analysis.

$\hat{Y}(X)$: The name of the regression equation (relationship) derived from regressing Y on X .

$\{\hat{Y}_i : i = 1, \dots, n\}$: Predicted designated test method results. The values computed from the $\{X_i\}$ and the regression equation, $\hat{Y}(X)$.

The designated method values, $\{Y_i\}$ (the dependent variable), should be regressed against the alternative method data, $\{X_i\}$ (the independent variable). Regressing Y on the alternative method data yields relationships for which the variability of predicted designated method results can be estimated by straightforward computations.

The remainder of this subsection discusses guidelines for statistical documentation of the regression relationship. Guidelines for computing estimates of the variability of predicted designated method values are discussed in the next subsection.

The following standard statistical documentation of the regression relationship must be provided:

1. A scatter plot of the paired $\{(X_i, Y_i) : i = 1, \dots, n\}$ with the regression relationship superimposed
2. A scatter plot of the paired \hat{Y}_i and Y_i
3. A scatter plot of residuals $(Y_i - \hat{Y}_i)$ vs. X
4. A normal probability or Q-Q plot of the residuals
5. An ANOVA table for the regression, the standard error, and the value of r^2 (the square of the correlation coefficient)
6. A table of the regression coefficients and their t -statistics and significance levels.
7. A computation of the uncertainty of the predicted Y values, as discussed in detail below

Evaluations of the following types are customarily included in evaluations of the merits of regression models. The evaluations should be supported by references to the above statistical documentation:

1. How well the relationship fits the data, with special attention to the fit at values of the fuel property near regulatory limits

2. The range of slopes of the regression function, documenting that it does not include excessively small and excessively large slopes which would make it impossible to relate predicted Y values to X values with acceptable precision
3. Comparison of the merits of the chosen functional form of the regression equation to the merits of other plausible functional forms, if appropriate (zero intercept vs. non zero intercept)
4. The homogeneity of the residuals and the absence of significant departures from normality of the residuals. Approximate normality of the residuals is important because the quantification of the uncertainty of the predicted values assumes normality

Petitioners are encouraged to submit any additional documentation that will help to support their conclusions about the merits of the regression model.

An Upper Bound on the Variability of the Differences $Y - \hat{Y}$

The previous subsection contained guidelines for documenting that the regression relationship, $\hat{Y}(X)$, derived from regression of the Y values for gasolines on the X data satisfactorily represents the relationship between each X and the average of the Y corresponding to those X data. A satisfactory regression relationship is necessary, but not sufficient, for an alternative method to be judged equivalent. In addition, the relationship between the X and Y data must be good enough that the predicted values of Y are unlikely to seriously deviate from the corresponding measured values of Y anywhere in the property range over which the alternative method is to be considered equivalent.

The variability of the differences between individual Y values and the corresponding predicted values, \hat{Y} , is a result of both the uncertainty in the regression relationship and the random variation inherent in the Y and X. Upper confidence bounds for both of these components of variability are taken into account in computing an upper bound that is expected to exceed at least 95% of future measured values, Y. This upper bound, $\hat{Y}_{\text{UTB}}(X)$, is to have a confidence level of 95%. The upper confidence bound is denoted by $\hat{Y}_{\text{UTB}}(X)$ because it varies with X. Details of these computations are given in Appendix B.

The difference $\hat{Y}_{\text{UTB}}(X) - \hat{Y}(X)$ is an upper confidence bound for the variability of the differences $Y - \hat{Y}(X)$. That is, it is an upper confidence bound on the variability of expected (future) differences between designated test method results and corresponding predicted values based on alternative method results. And, in some respects, it is analogous to test method reproducibility. $\hat{Y}_{\text{UTB}}(X) - \hat{Y}(X)$ must be less than or equal to the reproducibility of the designated test method for all values of X for which the alternative method is to be used.

In some cases, it would be more appropriate to use X instead of $\hat{Y}(X)$ as a predictor for Y . It is left to the petitioner to make that case in such instances.

The reproducibilities of many designated test methods are not constant but are a function of property level, or in the case of distillation properties, a function of the slope of the distillation curve. In cases where the reproducibility is not constant, it is left to the petitioner to determine how to deal with the issue. Petitioners should select a simple method for dealing with variable reproducibility. For example, the ARB will entertain (and has approved) petitions in which a "representative" value of reproducibility was used to determine whether or not $\hat{Y}_{\text{UTB}}(X) - \hat{Y}(X)$ was acceptably small over the range of X .

The stringency of the requirement on $\hat{Y}_{\text{UTB}}(X) - \hat{Y}(X)$ is a function of property range. If a site-specific alternative method were to be validated over a very narrow range of property values, the requirements listed above, including the requirement on $\hat{Y}_{\text{UTB}}(X) - \hat{Y}(X)$, would not by themselves be sufficient to ensure that the method measured the fuel property well. The additional requirement that the value of r^2 equal or exceed 0.8 gives assurance that the property would be well measured even if the alternative method were validated over a narrow property range. Somewhat smaller values might also suffice. In the event that r^2 is less than 0.8, the petitioner has the burden of justifying the smaller value.

APPENDIX B

COMPUTATION OF AN UPPER CONFIDENCE BOUND ON THE TOTAL VARIABILITY OF Y VALUES DERIVED FROM AN ALTERNATIVE METHOD

This appendix describes the three steps of the computation of an upper confidence bound, with some comments on alternative choices of bounds. This computation of an upper confidence bound assumes that a standard linear regression of Y on X has been computed.

Step 1

The variability of the regression of Y on X is quantified by an upper confidence band for the regression relationship. This confidence band, a function of X denoted by $\hat{Y}_{UCB}(X)$, must be an upper bound for the predictions of Y for *all* the relevant values of X . (Confidence bands with this property are often called simultaneous bands.) The confidence level of this band will be discussed in the paragraph on combining the two bounds.

There are numerous types of simultaneous upper confidence bands for standard linear regression functions. The use of any type of band that has the required simultaneity properties is acceptable. When there are a lot of data, the widths of bands of various types may not be very different. Simultaneous confidence bands differ in the following ways:

1. whether they may be computed only for certain functional forms of regressions
2. whether they are bands for only predictions from the regression function or bands for a more general class of functions
3. in their shapes
4. whether they are confidence bands for only a specified finite interval of independent variable values or for all values.

The more limited the situations in which a given type of band can be applied, the tighter the band will be. For example, Scheffe's¹ S-method bands are hyperbolic bands which may be computed for all linear regressions, but they are almost always broader than other types of bands because they are bands for a much more general class of functions for all values of the dependent variable. Near the other extreme, the bands derived by Bohrer and Francis² are the tightest possible hyperbolic upper confidence bands for the regression equation $\tilde{Y}_i = \beta_0 + \beta_1 X_i$ over a finite interval.

Step 2

The variability of the Y values about the average Y value predicted by the regression function, the residual variability of the regression model, is quantified

by its standard deviation, which is commonly called the standard error of the regression and denoted by σ . A one-sided upper confidence interval for the standard error σ is computed, assuming that $(n - 2)s^2/\sigma^2$ has a chi-squared distribution, as is the case for standard regression models. The upper confidence bound for σ is denoted by s_{UCB} . The confidence level of the interval will be discussed in Step 3. The upper bound for the variability of the Y values about the regression relationship, $1.645 * s_{UCB}$, is chosen to be the 95th-percentile of their distribution, with the standard deviation of this distribution assumed to be the upper confidence bound s_{UCB} . The confidence bound on the variability of Y values is thus a bound on the range of the lower 95% of these values.

Step 3

The confidence bound for the total variability of the Y values is the sum of the two previously computed bounds:

$$\hat{Y}_{UTB}(X) = \hat{Y}_{UCB}(X) + 1.645 s_{UCB}$$

The bound $\hat{Y}_{UTB}(X)$ is thus a curve parallel to the confidence bound $\hat{Y}_{UCB}(X)$ at the distance $1.645 s_{UCB}$ above it.

The desired 95% confidence level of $\hat{Y}_{UTB}(X)$ is demonstrated by appropriate choice of confidence levels and use of the Bonferroni method, as follows:

Let the confidence level of $\hat{Y}_{UCB}(X)$ be $100(1 - \alpha_1)\%$ and the confidence level of s_{UCB} be $100(1 - \alpha_2)\%$. Then the confidence level of $\hat{Y}_{UTB}(X)$ is at least $100(1 - \alpha_1 - \alpha_2)\%$, by the basic probabilistic inequality used in the Bonferroni method. For example, if α_1 and α_2 were both 0.025 (the usual choice), the confidence level of $\hat{Y}_{UTB}(X)$ would be at least $100(1 - 0.025 - 0.025)\% = 95\%$. α_1 and α_2 are not required to be equal.

$\hat{Y}_{UTB}(X) - \hat{Y}(X)$ must be less than R , the reproducibility of the designated test method for all values of X for which the alternative method is to be used.

Equations for $\hat{Y}_{UCB}(X)$ and $\hat{Y}_{UTB}(X)$

Paired alternative and designated method data are denoted by:

$$\{(X_i, Y_i) : i = 1, \dots, n\}$$

Linear Model with Nonzero Intercept

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i$$

where β_0 and β_1 are unknown constants and the $\{\varepsilon_i\}$ are random errors in the designated method results, $\{Y_i\}$. The errors are assumed to independently and normally distributed with the same standard deviation σ . The $\{X_i\}$ are assumed to be error free. The estimates of β_0 , β_1 , and σ are denoted by b_0 , b_1 , and s respectively.

The $100(1-\alpha)\%$ upper confidence bound $\hat{Y}_{\text{UCB}}(X)$ is given by:

$$\hat{Y}_{\text{UCB}}(X) = b_0 + b_1 X + B(\alpha, n) s \sqrt{\frac{1}{n} + \frac{(X - \bar{X})^2}{\sum (X_i - \bar{X})^2}}$$

where $B(\alpha, n)$ is a "Bohrer-Francis constant" (see reference 2) and n is the number of samples. \bar{X} is the mean of the $\{X_i\}$.

$$\hat{Y}_{\text{UTB}}(X) = b_0 + b_1 X + B(\alpha, n) s \sqrt{\frac{1}{n} + \frac{(X - \bar{X})^2}{\sum (X_i - \bar{X})^2}} + 1.645 s_{\text{UCB}}$$

Linear Model with the Zero Intercept

$$Y_i = \beta_1 X_i + \varepsilon_i$$

In this case, the one-sided upper confidence bound with confidence level $100(1-\alpha)\%$ is:

$$\hat{Y}_{\text{UCB}}(X) = bX + t(\alpha, n-1) s \sqrt{\frac{X^2}{\sum X_i^2}}$$

where $t(\alpha, n-1)$ is the value exceeded by $100\alpha\%$ of the "Student" t distribution with $n-1$ degrees of freedom.

$$\hat{Y}_{\text{UTB}}(X) = bX + t(\alpha, n-1) s \sqrt{\frac{X^2}{\sum X_i^2}} + 1.645 s_{\text{UCB}}$$

References:

1. Scheffe, H., Analysis of Variance, Section 3.5, Wiley, 1959
2. Bohrer, R. and Francis, G. K., "Sharp one-sided confidence bounds for linear regression over intervals", Biometrika 59, 1972, pp 99 – 107.