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A Single Model Procedure for Estimating Tank Calibration Equations

A. M. Liebetrau

October 1997

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Executive Summary

A fundamental component of any accountability system for nuclear materials is a tank calibration equation that relates the height of liquid in a tank to its volume. Tank volume calibration equations are typically determined from pairs of height and volume measurements taken in a series of calibration runs. After raw calibration data are standardized to a fixed set of reference conditions, the calibration equation is typically fit by dividing the data into several segments--corresponding to regions in the tank--and independently fitting the data for each segment. The estimates obtained for individual segments must then be combined to obtain an estimate of the entire calibration function. This process is tedious and time-consuming. Moreover, uncertainty estimates may be misleading because it is difficult to properly model run-to-run variability and between-segment correlation.

In this paper, we describe a model whose parameters can be estimated simultaneously for all segments of the calibration data, thereby eliminating the need for segment-by-segment estimation. The essence of the proposed model is to define a suitable polynomial to fit to each segment and then extend its definition to the domain of the entire calibration function, so that it (the entire calibration function) can be expressed as the sum of these "extended" polynomials. The model provides defensible estimates of between-run variability and yields a proper treatment of between-segment correlations.

A portable software package, called TANCS, has been developed to facilitate the acquisition, standardization, and analysis of tank calibration data. The TANCS package was used for the calculations in an example presented to illustrate the unified modeling approach described in this paper. With TANCS, a trial calibration function can be estimated and evaluated in a matter of minutes.

Acknowledgment

This document was originally prepared as a paper for presentation at the IAEA Symposium on International Safeguards held on 13-17 October, 1997. It is being made available as a technical report because the presentation was canceled by the sponsor on the eve of the conference and the paper was withdrawn.

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1. INTRODUCTION

The calibration equation that relates the height of liquid in a tank to its volume is a fundamental component of any accountability system for nuclear materials. Tank volume calibration equations are typically estimated from pairs of height and volume measurements taken in a series of calibration runs. The data must be standardized to a fixed set of reference conditions to ensure that comparability has not been lost because of varying ambient conditions during the calibration exercise.

A comprehensive model for standardization of tank calibration data was presented at a previous IAEA Symposium. [1] The model is based on the American National Volume Standard ANSI N15.19-1989. [2] Documents that describe the methods of ANSI N15.19, or extensions thereof, are being drafted by an International Standards Organization working group, with the expectation that they will eventually be adopted internationally. Details of the data standardization model are not discussed further here; the interested reader is directed to the references cited above.

Estimates of tank calibration equations have traditionally been constructed by dividing the data into several segments--corresponding to regions in the tank--and independently fitting the data for each segment. The estimates obtained for individual segments must then be combined to obtain an estimate of the entire calibration function. This process is tedious and time-consuming. Moreover, uncertainty estimates for each segment are obtained independently of the data in adjacent segments, although in actuality data from adjacent segments are certainly not independent.

With high-precision measurement systems, tank volume calibration data from several runs typically exhibit significant run-to-run variability. Unless between-run variability is modeled properly, the variability estimates for volume measurements can be seriously in error. For example, when significant between-run variability is ignored in the statistical analysis, actual measurement variability can be seriously underestimated. In a recent paper, Liebetrau and Thomas present a model that yields reasonable estimates of uncertainty regardless of whether or not between-run variability is significant. [3]

In this paper, we describe a generalization of the Liebetrau-Thomas model for which all model parameters can be estimated simultaneously for all segments of the calibration data, thereby eliminating the need for segment-by-segment estimation. As with other estimation procedures, the first step is to identify suitable calibration segments and define polynomials of suitable degree to fit each. Then, the polynomial for each segment is extended over the entire domain of the calibration function so that the function can be expressed as the sum of these "extended" polynomials. This permits estimation of the entire calibration function in a single mathematical calculation. Moreover, segment-to-segment correlations among observations are automatically incorporated into variability estimates, because the fitting procedure employs all of the data.

The proposed fitting model is described in Section 2, uncertainty estimation is discussed in Section 3 and an example is presented in Section 4, and conclusions are drawn in Section 5.

2. MODELING APPROACH

The essence of the approach described here for simultaneously estimating the entire calibration function is to view the calibration functions for individual segments as functions that extend over the entire range of the calibration function, rather than as functions restricted to the segment on which they are originally defined. The "trick" is to write the function for each segment so that the desired calibration function can be written as the sum of these individual functions over its entire domain. Once this is accomplished, standard statistical procedures can be used to estimate the entire calibration function in a single mathematical calculation.

2.1 Model Construction

The basic idea of the construction is illustrated by means of the example shown in Figure 1. Figure

1(a) shows "typical" calibration data from a three-segment calibration function f . The variables x and y denote volume and height, respectively. Segment boundaries are denoted by c_1 and c_2 . Figure 1(b) shows a function f_1 that is linear in the first segment ($x \leq c_1$) and constant (with value $f_1(c_1)$) throughout the remaining two segments. Figure 1(c) shows a function f_2 that is zero in the first segment ($x \leq c_1$), linear in the second segment ($c_1 < x \leq c_2$), and constant (with value $f_2(c_2)$) in the third segment ($c_2 < x$). Finally, Figure 1(d) shows a function f_3 that is zero in the first two segments and linear in the third. The calibration function f can now be expressed over its *entire range* as the sum of the functions f_1 , f_2 , and f_3 :

$$f(x) = f_1(x) + f_2(x) + f_3(x), \text{ valid for all } x$$

The result is shown in Figure 1(e).

The construction illustrated in Figure 1 makes it possible to write a design matrix that permits all fitting to be done in a single mathematical calculation. In matrix notation, the calibration model is

$$Y = G\beta + \varepsilon \quad (1)$$

where

Y is an $n \times 1$ vector of observed (standardized) heights,
 G is an $n \times p$ design matrix whose individual elements are functions of observed (standardized) volumes,
 β is a $p \times 1$ vector of model parameters, and
 ε is an $n \times p$ vector of errors.

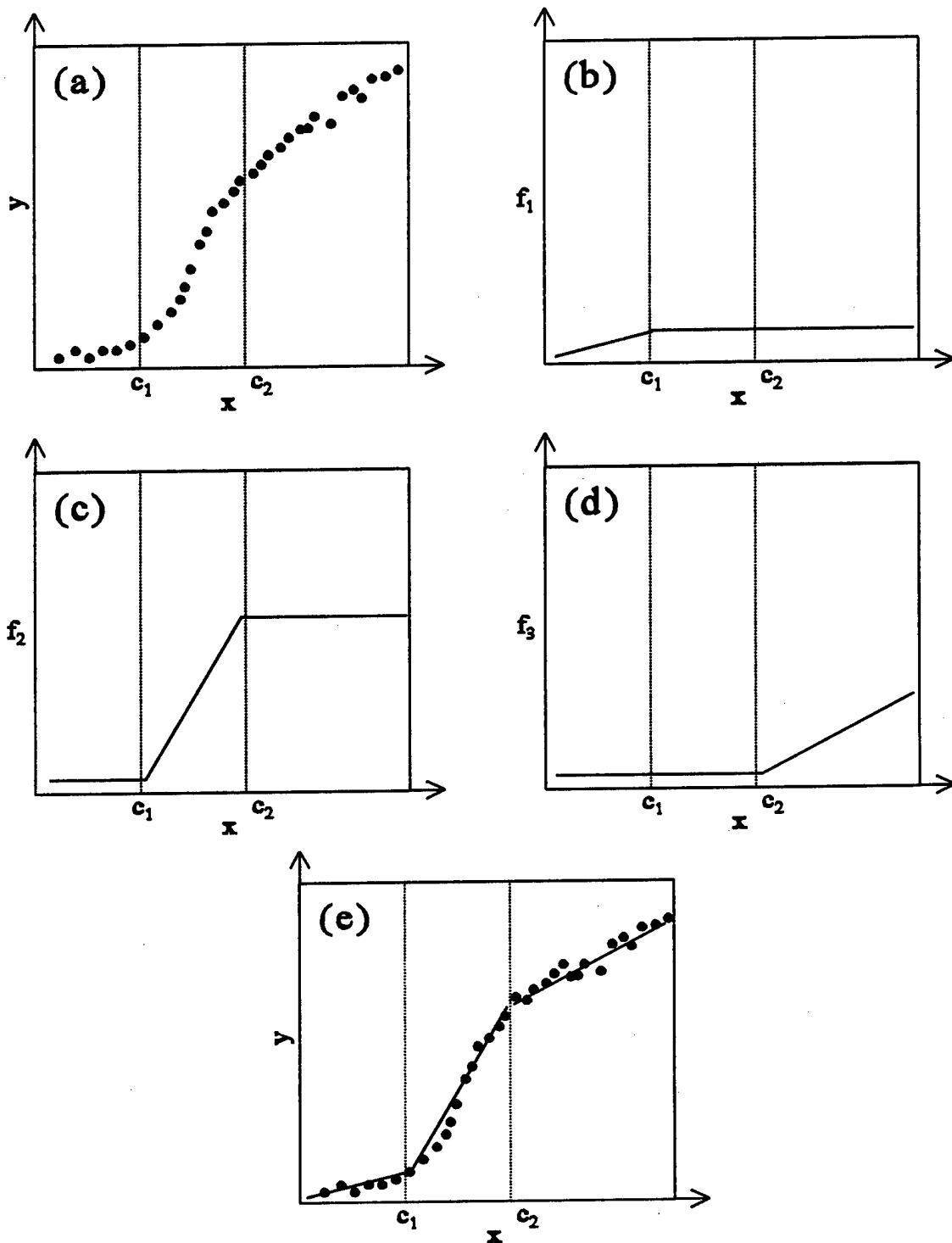


Figure 1. Three-Segment Illustration of the Modeling Construct. "Typical" calibration data is shown in (a). Extensions of the functions that fit each segment of the data are shown in (b), (c), and (d), respectively. Their sum, which fits the entire calibration function, is shown in (e).

The components of ε are assumed to be independent and identically distributed random variables, each with mean zero and standard deviation σ . The first column of G represents the intercept term; each remaining column represents a term in a polynomial expression selected to model the calibration function f over a particular segment. The design matrix for the three-segment example of Figure 1 has four columns: one for the intercept and one for the linear term in each segment. The last three columns of G correspond, respectively, to the slopes of the linear segments of f_1 , f_2 , and f_3 .

Individual columns of G that correspond to linear functions are constructed as follows. If a segment has boundaries c_{k-1} and c_k , then the column contains a zero for each observation for which $x \leq c_{k-1}$. For each observation x in the given segment¹ (i.e., for which $c_{k-1} < x \leq c_k$), the column contains the value $(x - c_{k-1})$. For observations for which $x > c_k$, the column contains the value $(c_k - c_{k-1})$. Thus, in this illustrative example, the design matrix has the block diagonal form

$$G = \begin{bmatrix} 1 & x - c_0 & 0 & 0 \\ 1 & c_1 - c_0 & x - c_1 & 0 \\ 1 & c_1 - c_0 & c_2 - c_1 & x - c_2 \end{bmatrix}$$

The basic idea can easily be extended to calibration functions comprised of more than three segments and to cases where the functions f_i are polynomials of higher degree. If a segment of the calibration function is to be fit with a quadratic polynomial, for example, the design matrix will have one column for the linear term and a second column for the quadratic term. The column for the linear term is constructed as in the illustrative example of Figure 1. Entries in the column for the quadratic term are obtained by squaring the corresponding entries in the column for the linear term. Design matrices can be constructed in an analogous fashion for models which include higher-degree polynomials.

After the segment boundaries c_k are defined and the degree of the polynomial for each segment is specified, the design matrix G can easily be generated by computer.

2.2 Run-to-Run Fluctuations

The model described in the previous section can be extended to account for run-to-run fluctuations in model parameters. Let

$$Y_r = G_r(\beta + \theta_r) + \varepsilon_r \quad (2)$$

where r designates the run number and the quantities Y_r , G_r and ε_r are defined as in Equation (1), except that they pertain only to the run r . Thus,

¹The lower boundary of the first segment is denoted by $c_0=0$.

Y_r is an $n_r \times 1$ vector of observed heights from run r ,
 G_r is an $n_r \times p$ design matrix whose individual elements are functions of observed volumes
(The rows of G_r are the rows of G that involve observations from the run r),
 β is a $p \times 1$ vector of model parameters, and
 ε_r is an $n_r \times p$ vector of errors.

As with the parent model, the components of ε are assumed to be independent and identically distributed random variables, each with mean zero and standard deviation σ .

The quantity θ_r is a $p \times 1$ vector of parameters that represent fluctuations in the corresponding parameters of β that are attributable to run r . The components θ_{rj} of θ_r are assumed to be independent random variables, each with mean zero and standard deviation ϕ_j . The parameters ϕ_1 to ϕ_p describe the run-to-run variability for corresponding model parameters (i.e., intercepts and slopes).

The parameters in the model of Equations (1) and (2) are estimated using the method of moments, which is quick and comparatively simple. The first step is to calculate the residual sum of squares (RSS) for a sequence of models. The RSS for the i th model, denoted RSS_i , is obtained by fixing the first i parameters of β and allowing the remaining parameters to vary. (In effect, the parameters θ_{rj} are constrained to be zero for $j \leq i$). It can be shown that (i) the expected value of RSS_i (from the model with no constrained parameters) is a function of σ ; and (ii) differences between residual sums of squares RSS_i are functions of the standard deviations σ and ϕ_j . After appropriate models are fitted, estimates of components of β and ϕ are obtained by equating the observed values of σ and ϕ_j with their expected values, and solving the resulting set of equations.

There are several ways to carry out the estimation. The model $i=0$, in which every parameter is allowed to vary, is fit first. One approach is to separately fit the data from each run r to obtain estimates of $\beta_r = (\beta + \theta_r)$; and then the average of all values β_r can be used to estimate β . Alternatively, the parameters β can be estimated by fitting a model in which corresponding intercept and "slope" parameters are constrained to be equal across all runs. The two procedures yield slightly different estimates, but differences between the two methods will generally have a negligible effect on results.

The estimation procedure proposed here is an extension of the one developed by Liebetrau and Thomas [3] in several senses. First, fitting a function to several segments is accomplished in a single mathematical step. Second, the present procedure easily allows the fitting of polynomials of higher degree. Third, all parameters are estimated jointly using all of the data, so that segment-to-segment correlations are automatically incorporated into uncertainty estimates. Finally, the representation described here does not require the assumptions made in [3] (to simplify the computation) that the vector of volume measurements is the same for all runs.

3. UNCERTAINTY ESTIMATION

Estimates of the parameters β are uncertain because of two factors: uncertainty in the observational errors ϵ and run-to-run fluctuations θ_r . The run-to-run differences are relevant not only because they appear in the existing calibration data, but also because they will be present in any future observations made to estimate volumes. With some degree of confidence, one can construct a region for the true calibration function, for the difference between two estimates of the calibration function, and for individual observations from a single (new) calibration run.

3.1 General Approach

The variance-covariance matrix of the estimated vector of parameters $\hat{\beta}$ can be estimated in the following way. If $\hat{\beta}_r$ is the vector of estimated parameters for run r , then let

$$\hat{\beta} = R^{-1} \sum_{r=1}^R \hat{\beta}_r$$

where R is the total number of runs. By applying a basic property of conditional expectation, it follows that

$$\begin{aligned} \text{Var}(\hat{\beta}) &= E\left[\text{Var}(\hat{\beta}|\theta_r, r=1, \dots, R)\right] + \text{Var}\left[E(\hat{\beta}|\theta_r, r=1, \dots, R)\right] \\ &= E\left[R^{-2} \sum_{r=1}^R \text{Var}(\hat{\beta}_r|\theta_r)\right] + \text{Var}\left(\beta + R^{-1} \sum_{r=1}^R \theta_r\right) \\ &= \sigma^2 R^{-2} \sum_{r=1}^R (G_r^T G_r)^{-1} + R^{-1} I \Phi^2 \end{aligned} \quad (3)$$

In Equation (3), I is the $p \times p$ identity matrix, where p is the number of parameters in the vector β , and Φ^2 is a vector containing the run-to-run variance parameters ϕ_j^2 (ϕ_j^2 is the variance of θ_j). The final term in Equation (3) shows explicitly how run-to-run variability contributes to the variance of $\hat{\beta}$. The expression in Equation (3) can be estimated by replacing the variances σ^2 and ϕ_j^2 with their estimates.

All of the confidence regions are based upon the variability of the predicted calibration curve

$$g_h \hat{\beta}$$

where g_h is the row of the design matrix (a row vector) that corresponds to a hypothetical observation x_h . The variance of this observation is

$$a^2 = g_h \text{Var}(\hat{\beta}) g_h^T \quad (4)$$

Various confidence regions can be calculated from Equation (4) following methods described in [4]. The variance a^2 is a linear combination of the variance estimates σ^2 and $\hat{\phi}_j^2$, so its distribution can be approximated by a Chi-square distribution. The approximate degrees of freedom (df) for the distribution of a^2 can be computed using the Welch-Satterthwaite method. [5] For this calculation, the estimate of σ^2 is assumed to have a Chi-square distribution with $(N-Rp)$ degrees of freedom, where N denotes the total number of observations in all runs, and each component of Φ^2 is assumed to have a Chi-square distribution with $(R-1)$ degrees of freedom.

It is also possible by means of the Welch-Satterthwaite method to derive estimates for the degrees of freedom for σ^2 and $\hat{\phi}_j^2$ from the data, and use these estimates to determine the degrees of freedom for a^2 . However, calculations for this approach are more complicated and in examples we have considered, differences between the two methods are generally negligible.

3.2 Confidence Regions

Confidence regions are given here for the true calibration function, for the difference between two estimates of the calibration function, and for future individual height measurements. All are based on Equation (4) and all are derived using methods presented in [6].

3.2.1 True Calibration Function

Approximate $100(1-2\alpha)\%$ confidence bounds on the true calibration function at some volume x_h are given by

$$g_h \beta \pm a (pF_{p,v}^\alpha)^{0.5} \quad (5)$$

where α is a specified significance level (e.g., 0.025 or 0.05), v is the approximate degrees of freedom for the variance estimate a^2 and $F_{p,v}^\alpha$ is the $100(1-\alpha)$ th percentage point from the F-distribution with degrees of freedom p and v .

Confidence bands for the entire calibration function may be obtained by plotting the confidence bounds calculated from Expression 5 for a series of values of x_h .

3.2.2 Difference Between Two Calibration Functions

Approximate $100(1-2\alpha)\%$ confidence bounds on a confidence region for the difference between a new calibration function, estimated from a single new run, and an existing calibration function are given by

$$g_h (\beta - \beta_{new}) \pm [(a^2 + \sigma_{new}^2 g_h G_{new} g_h^T + \sum_{j=1}^p g_{hj}^2 \hat{\phi}_j^2) pF_{p,v}^\alpha]^{0.5} \quad (6)$$

where v is the approximate degrees of freedom for the quantity

$$a^2 + \sigma_{new}^2 z_h Z_{new} z_h^T + \sum_{j=1}^p g_{hj}^2 \phi_j^2 \quad (7)$$

In Expressions (6) and (7), expressions for the design matrix, parameter estimates, and variance estimate for the new calibration run are denoted by Z_{new} , $\hat{\beta}_{new}$, and σ_{new}^2 , respectively. The three terms in Expression (7) correspond to the error in the estimation of $\hat{\beta}$, the error in estimating $\hat{\beta}_{new}$, and the fluctuations θ_{new} of the new run, respectively. As in previous cases, the degrees of freedom v is calculated using the Welch-Satterthwaite method. [5]

Confidence bands for the difference between the two calibration functions, plotted for a series of values of x_h , can be used to compare the two functions. If at any point, the confidence region for the difference between the new and existing calibration functions does not contain zero, differences between the two functions are significant at the specified significance level.

3.2.3 Tolerance Bounds for Individual Height Measurements

Approximate $100(1-\alpha)\%$ tolerance bounds with coverage probability p for individual height measurements are given by

$$g_h \hat{\beta} \pm \left\{ \left[\left(a^2 + \sum_{j=1}^p g_{hj}^2 \phi_j^2 \right) \left(p F_{p+1, v}^\alpha \right) \right]^{0.5} + z_{p/2} \left[\frac{\xi}{X_\xi^2 \left(\frac{\alpha}{2} \right)} \right]^{0.5} \right\}$$

where v is the approximate degrees of freedom for the quantity

$$a^2 + \sum_{j=1}^p z_{hj}^2 \phi_j^2$$

and $z_{p/2}$ and $\chi^2(\alpha/2)$ are percentage points for the standard normal distribution and the chi-square distribution with ξ degrees of freedom, respectively. These tolerance bands are suitable for evaluating the variability of future new observations of liquid height.

4. EXAMPLE

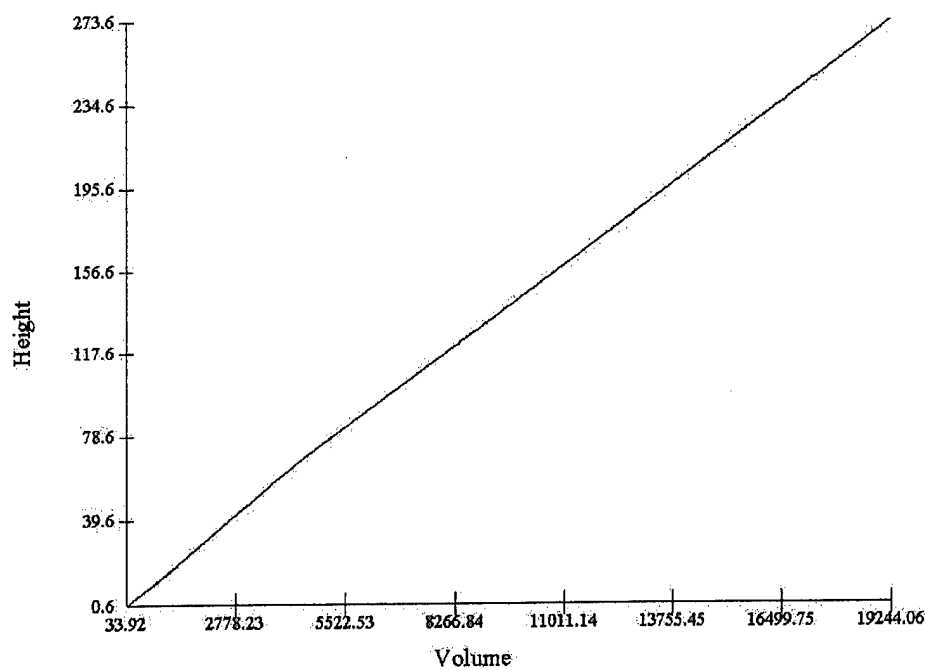
Figure 2a is a plot of liquid height vs. cumulative volume for data from six calibration runs on a large input tank at the Hanford facility. The nominal capacity of the tank is approximately 5000 gallons (19,000 liters), and its height is approximately 9 feet (2.75 m). The data were acquired during several calibration exercises conducted over a 10-year period. Each calibration run contains approximately 200 points.

Figure 2b shows a profile plot of the data shown in Figure 2a. The profile plot, which is obtained by plotting the residuals of a linear least-squares fit to the data from all runs, clearly shows features of the tank profile that cannot be seen at the scale of Figure 2a. The profile of the tank is quite well resolved because of the comparatively large number of calibration increments in each run. Note that the vertical scale in Figure 2b ranges from approximately -3 to 2, whereas the original measurements ranged from 0 to 275. The profile plot shows that in its lower region, the tank's cross-sectional area increases faster than average with volume. At about 5000 liters, the cross-sectional area of the tank begins to increase more slowly and remains more-or-less constant thereafter. The larger than average increase in the lower region is due to the internal tank structures, such as agitators and heating coils.

It is clear from Figure 2b that an improved fit to the data can be obtained by dividing it into two segments and fitting each separately (each fit can be regarded as an estimate of the tank's calibration function). Figure 3 shows the result of dividing the data into two segments at 4600 liters and fitting a linear function to the data of each segment. At capacity (275mm), the relative half width of the associated confidence intervals is approximately 0.07% ($\pm 0.2 \div 275$). Notice that the range on the vertical scale has been reduced from the previous fit by approximately an order of magnitude. The confidence intervals shown in Figure 3b were obtained with the methods described in Section 3, which confirm that run-to-run fluctuations are the largest source of variability. The two straight lines in the profile plot can be regarded as an initial estimate of the tank's calibration function. However, the residual plot in Figure 3b shows a great deal of structure that is not resolved by the two-segment fit.

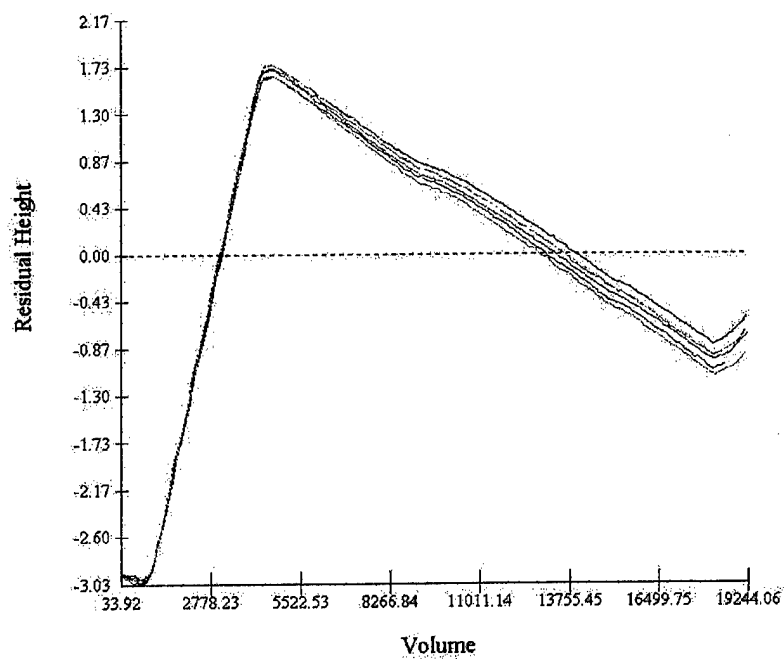
A more refined fit is shown in Figure 4. The fit consists of 7 segments: segment boundaries are indicated by vertical lines in the plot. A linear function is fit to the data of each segment. At capacity, the half width of the corresponding confidence intervals in this case is approximately the same as for the previous fit, but the fit is markedly improved. Some structure (in addition to the run-to-run differences) still remains in the residuals, so still more refined fits are possible. However, at some point in this fitting process, the reduction in variability becomes insignificant and further fitting will not improve the estimate of the tank's calibration function.

All the plots shown in this example were produced with a tank calibration software package, called TANCS. The TANCS package was designed to facilitate the acquisition, standardization and analysis of tank calibration and volume measurement data. With this code, trial estimates of a tank calibration function can be developed and evaluated in a matter of several minutes. The TANCS package was developed at the Pacific Northwest National Laboratory and is currently being used by the International Atomic Energy Agency.



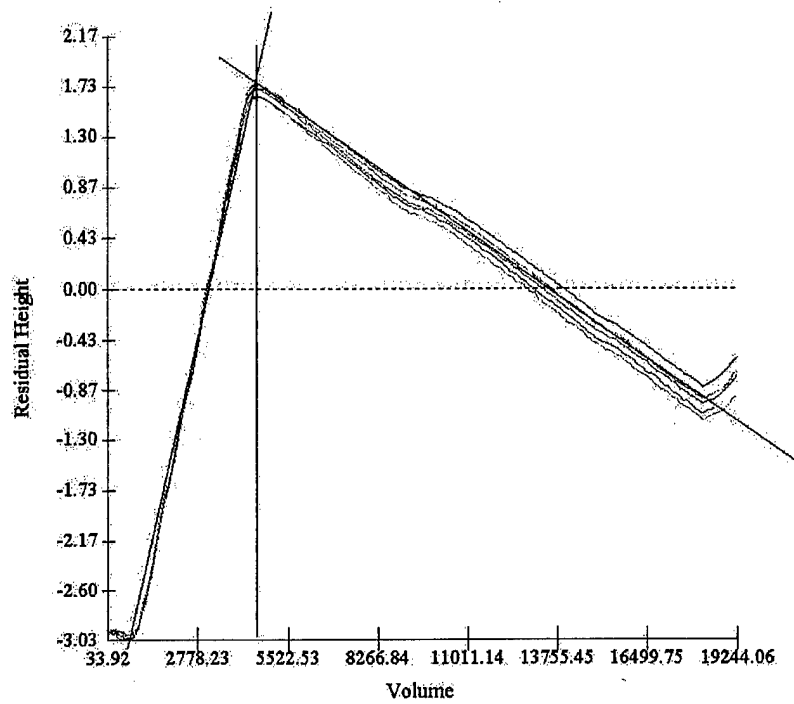
(a)

Profile Plot

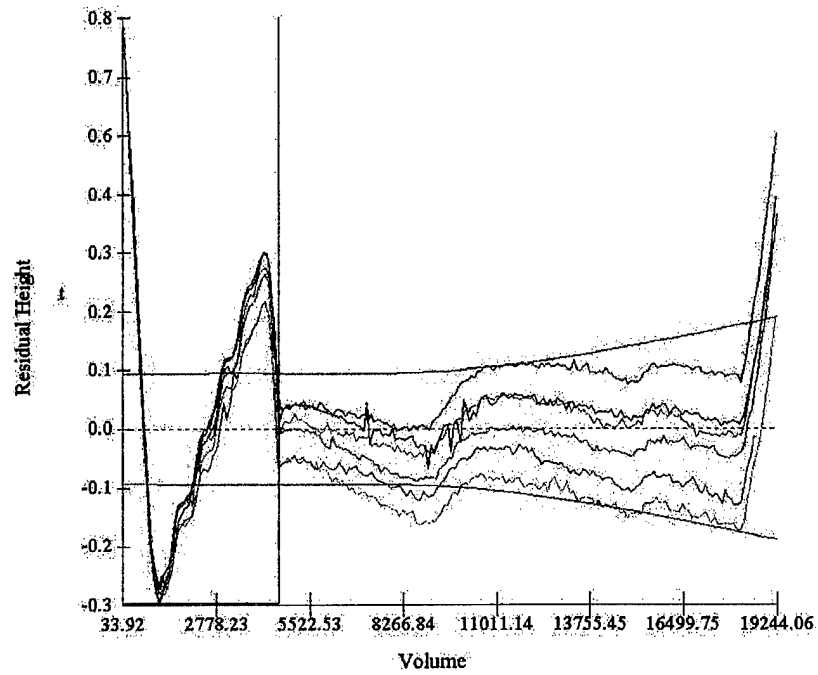


(b)

Figure 2. Cumulative (a) and Profile (b) Plots of Data from Six Calibration Runs

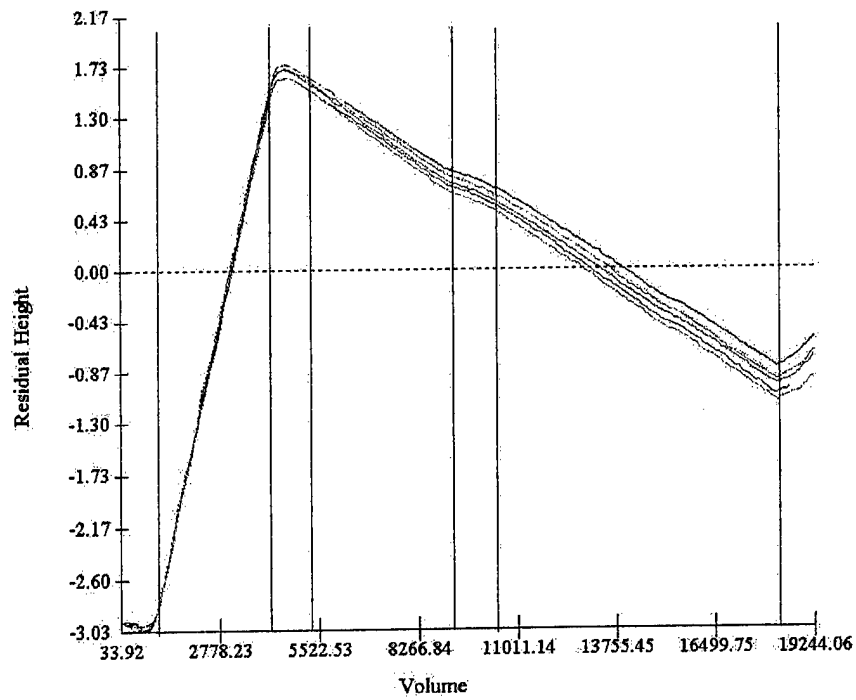


(a)

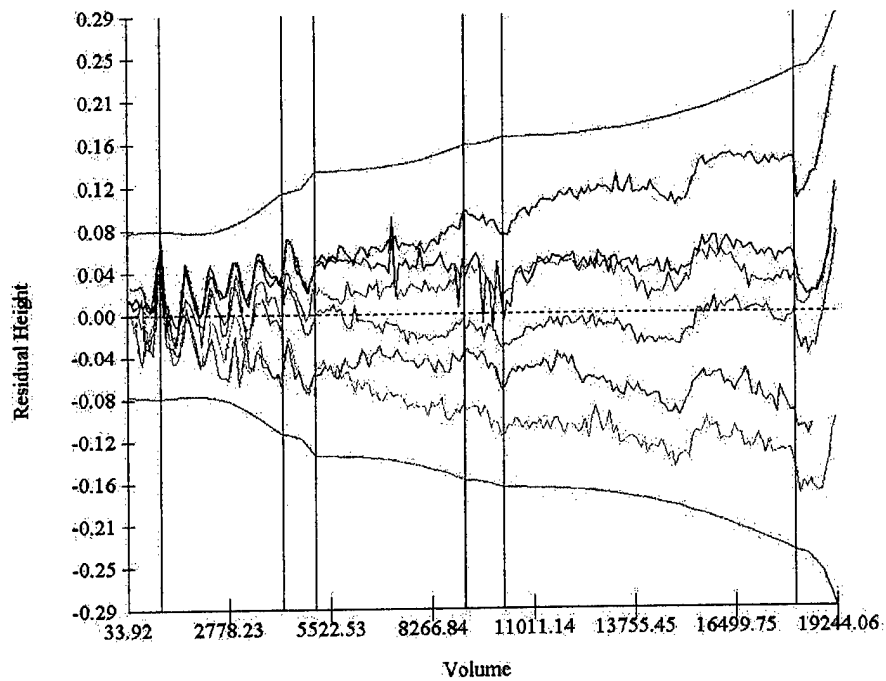


(b)

Figure 3. Trial Two-Segment Estimate of the Calibration Function (a) and Residuals Plot (b).



(a)



(b)

Figure 4. Refined Seven-Segment Estimate of the Calibration Function (a) and Residuals Plot (b)

5. CONCLUDING REMARKS

This report presents a method for estimating tank calibration equations that eliminates many of the difficulties associated with the traditional piecewise fitting approach. Most importantly, the model provides a defensible procedure for including the effect on variance estimates of run-to-run variability and segment-to-segment correlations. Moreover, with the proposed fitting approach, the calibration function can be fit in a single mathematical operation, which eliminates the need to combine independent fits for several segments. As an added benefit, the resulting estimate is automatically continuous at the specified cut points. Finally, a software package, called TANCS, has been developed that permits the user to standardize a set of raw calibration data, and create and examine a trial fit in a matter of minutes. The TANCS program was developed at the Pacific Northwest National Laboratory for the IAEA under the U.S. Program of Technical Support to International Safeguards. Additional information about the TANCS program is available from the author.

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