

**SPLINE REGRESSION MODELS  
FOR CALIBRATION DATA**

by

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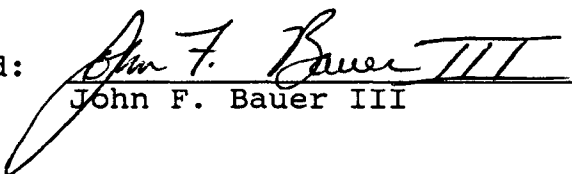
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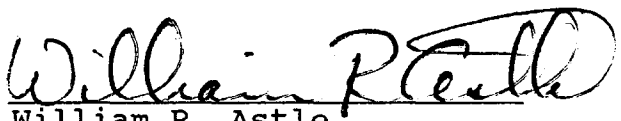
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**ABSTRACT**

By using splines to model calibration data for processing tanks which have varying internal structure, highly accurate calculations of the liquid content of such tanks can be obtained. This modeling procedure divides the processing tank into calibration segments and the respective data is fit with piecewise polynomials. The optimal least-squares estimates for this type of model can be obtained with the use of a non-linear regression method. By using this method, the volume of material in a processing tank can be more accurately calculated than by methods which use a linear model to fit the entire calibration data set. Volume calculations and a method to determine their uncertainties is discussed. Criteria are also established for determining what to do with historical calibration data when recalibrating a processing tank. Sample results are shown and discussed.

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## CHAPTER 1

### INTRODUCTION

Accurate calibration of processing tanks is necessary in the nuclear industry to support control and accountability programs for the nuclear materials. Volume measurements of the liquid material in such tanks must be determined to high accuracy as a part of the regular inventory control system.

A processing tank of special interest is one in which the interior is filled with components whose physical structure resembles that of a napkin ring. These rings are made up of a particular chemical content which will stabilize the liquid being stored in the tank. A major problem with the ring-filled tank is that as the rings shift, break, or compact, the internal structure of the tank may change. The varying internal structure of these tanks requires advanced calibration techniques to determine volume content with high accuracy. A general schematic of the ring-filled tank configuration is shown in Figure 1.1.

The calibration process described in this paper is intended to determine an accurate relationship between a processing tank's liquid measurement response (liquid height in a sight gauge) and the volume of its liquid content. The resulting calibration function is subsequently used to

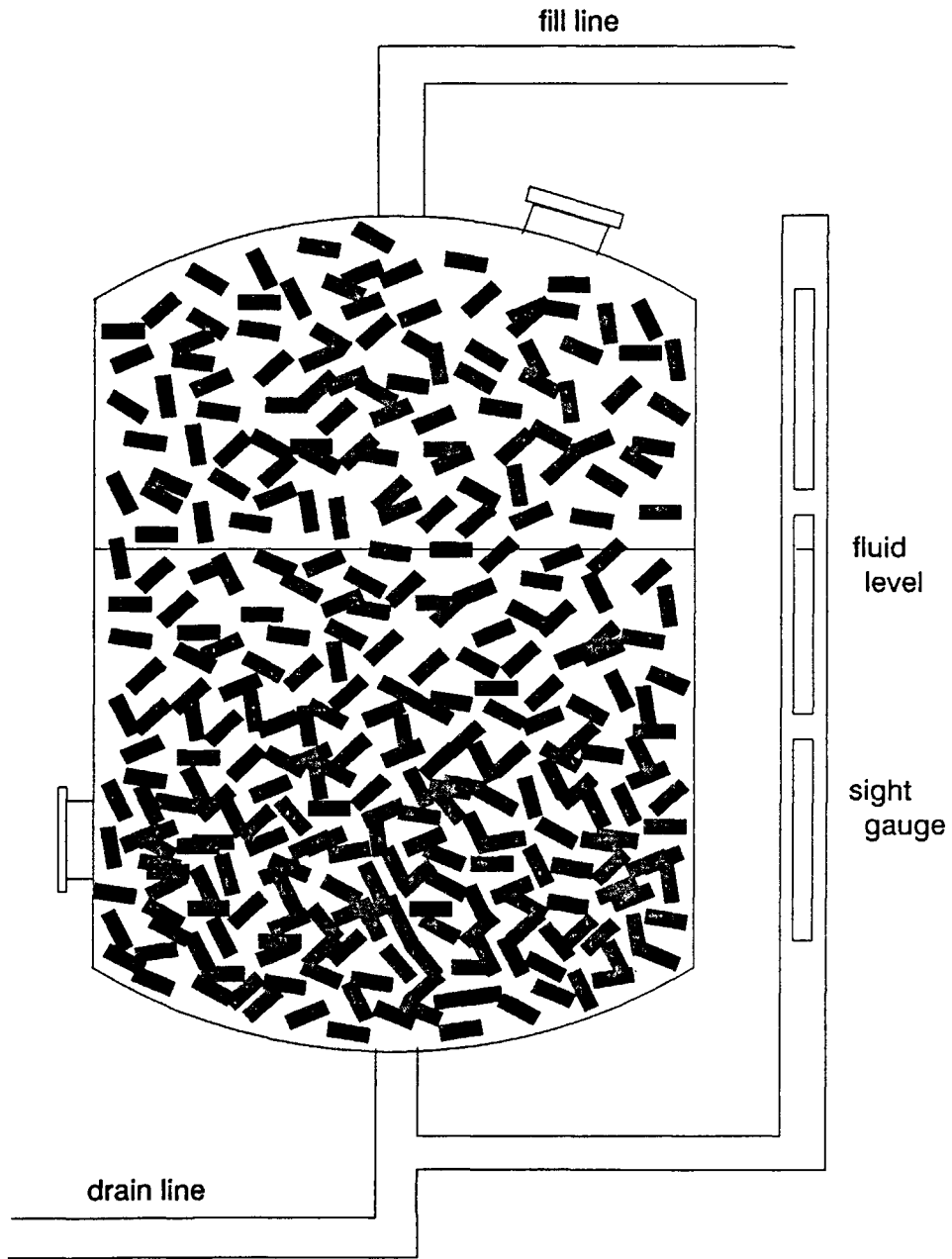


FIGURE 1.1 Tank Configuration

determine the liquid content of a ring-filled tank from a liquid height reading.

This paper will apply advanced tank calibration modeling techniques to ring-filled tank calibration data. Volume calculations and their associated uncertainties will be discussed. Additional criteria will also be established on how to incorporate historical calibration data when recalibrating a ring-filled tank. The typical procedures used for the collection of calibration data will remain unchanged.

## CHAPTER 2

### CALIBRATION PROCEDURE

A calibration run involves making a series of additions of known volumes of calibration liquid to the processing tank, and after each addition, recording the height of the liquid in the sight gauge on the tank (see Figure 1.1). Steps involved in performing a typical calibration run are listed as follows:

1. Preparatory steps, such as isolating, flushing, and draining the tank, are completed.
2. Initial steps, such as determining the initial tank volume, and recording data on both reference and ambient conditions, are accomplished.
3. The volumetric prover is filled with calibration liquid.
4. Prover-related data that include the volume of the calibration increment and temperature of the prover are recorded.
5. The liquid is transferred from prover to tank and appropriate times are allowed for drainage.
6. Conditions in the tank are allowed to stabilize. Steps such as mixing and waiting for the release of trapped gas, are taken to ensure that physical

properties of the tank liquid are uniform.

7. Data are acquired on the contents of the tank. The height of the liquid in the sight gauge, and the temperature and density of the tank liquid are recorded.
8. Repeat steps 3 through 7 for each calibration increment until the region of interest in the tank has been filled. (American National Standards Institute 1989)

A typical calibration consists of several calibration runs. This allows for analysis of within run and between run variability. However, other constraints such as time and cost do not always allow for several calibration runs. Another limiting factor in the number of calibration runs to be made is the generation of waste involved with each calibration run.

For a clean tank which has not been in production, the calibration liquid does not become a hazardous waste after passing through the tank. This allows for more than one calibration run to be made. However, once a tank has been in production, the calibration liquid which passes through the tank becomes a hazardous waste. Thus, to minimize the amount of hazardous waste being generated, a minimum number recalibration runs are made. The current practice for the

ring-filled tanks is to make only one calibration run during recalibration. For this reason, it is very important that there are no errors in the collection of the recalibration data.

For the calibration data used in this paper, the following assumptions are made:

1. The data is temperature corrected.
2. The liquid in the processing tank and the sight gauge is well mixed and of the same density.
3. The height of the liquid in the sight gauge is equivalent to the height of the liquid in the tank.
4. The initial volume in the tank is equivalent for all of the calibration runs.

**CHAPTER 3**  
**PRELIMINARY DATA ANALYSIS**

When a processing tank has a constant cross-sectional area, the calibration equation is simply a single straight line. However, the interiors of most processing tanks (especially ring-filled tanks) do not generally conform to idealized geometrical shapes, and thus have varying cross-sectional area. For modeling purposes, processing tanks can be considered to be composed of segments for which an idealized calibration equation is a good representation. Whenever possible, the segments in the tank are selected so that the cross-sectional area within each is either constant or changes in a well defined manner.

An initial step in developing the calibration model is to identify the calibration segments within the processing tank. Diagnostic plots such as profile plots and incremental slope plots are excellent tools for this purpose.

A profile plot is obtained by fitting a linear function,

$$H = a + bV \qquad (3.1)$$

where  $H$  is the liquid height measured in the sight gauge, in centimeters, and  $V$  is the cumulative volume added to the

tank, in liters, to the calibration data and then plotting the residuals versus the cumulative volume. This plot is basically the same as a plot of the liquid height measured in the sight gage versus cumulative volume with an expanded ordinate scale. A profile plot will graphically show the change in a tank's cross-sectional area. A straight line pattern on the profile plot indicates constant cross-sectional area, while abrupt changes indicate transition areas for calibration segments. An example of a profile plot for the calibration data of September 1989 from Table A-1 in Appendix A is shown in Figure 3.1.

An incremental slope plot is a plot of the point-to-point slopes of the calibration data versus the cumulative volume. In other words, the incremental slopes

$$b_i = (H_i - H_{i-1}) / (V_i - V_{i-1}) \quad (3.2)$$

where  $H_i$  is the height measured in the sight gauge in centimeters and  $V_i$  is the cumulative volume measured in liters, are plotted against  $V_i$ , for all calibration increments in the calibration run. This plot will show the changes in cross-sectional area of a tank in microscopic detail. Transition regions are identified by large differences in adjacent incremental slopes which are produced by abrupt



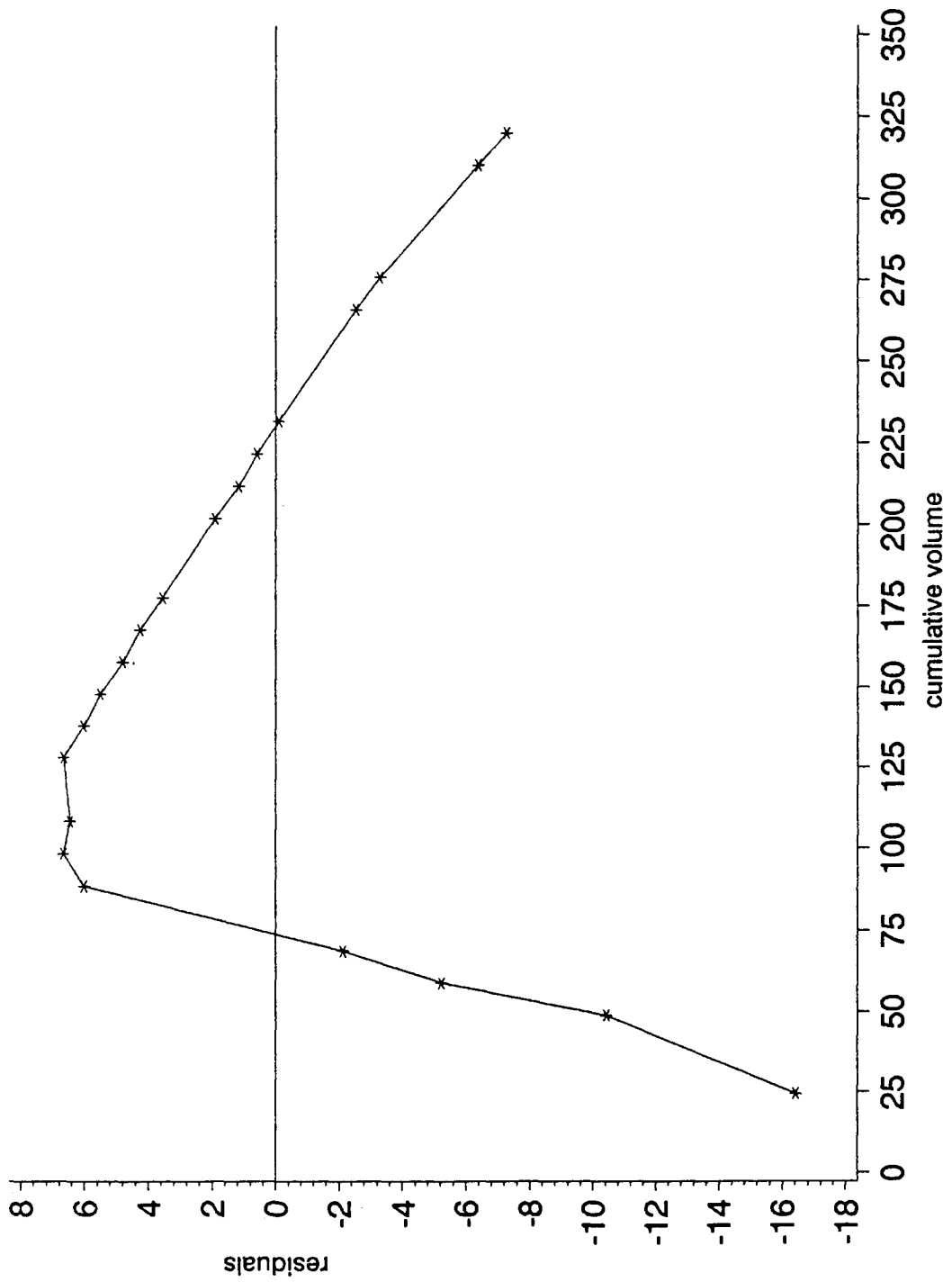


FIGURE 3.1 Profile Plot  
Calibration data from September 1989

changes in cross-sectional area. An example of an incremental slope plot for the calibration data of September 1989 from Table A-1 in Appendix A is shown in Figure 3.2.

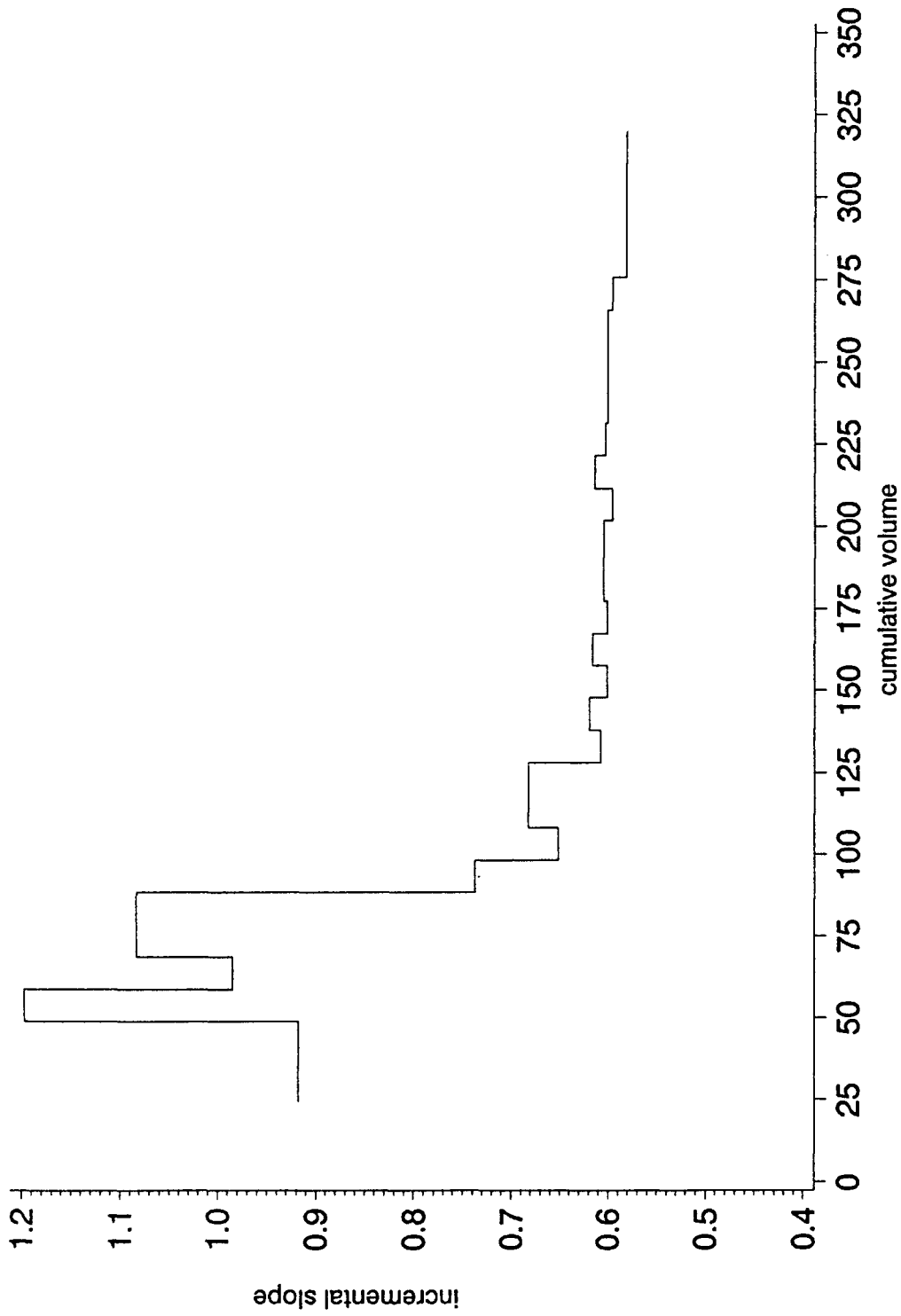


FIGURE 3.2 Incremental Slope Plot  
Calibration data from September 1989

**CHAPTER 4**  
**MODELING THE DATA**

Once the calibration segments and the approximate locations of the transition regions in the processing tank have been identified, a spline function can be used to fit the calibration data. A definition of a spline model is given as follows:

Splines are generally defined to be piecewise polynomials of degree  $n$  whose function values and first  $n - 1$  derivatives agree at points where they join. The abscissas of these joint points are called knots. Polynomials may be considered a special case of splines with no knots, and piecewise polynomials (sometimes also called grafted or segmented polynomials) with fewer than the maximum number of continuity restrictions may also be considered splines. The number and degrees of polynomial pieces and the number and position of knots may vary in different situations. (Smith 1979)

The "+" function facilitates the implementation of spline regressions. The "+" function is defined for the variable  $v$  as follows:

$$(v - k)^+ = (v - k) \text{ if } v - k > 0$$

$$(v - k)^+ = 0 \text{ if } v - k \leq 0$$

In this section an example of a spline function of degree two with only one knot is presented. First, assume the position of the knot is known. Thus, the spline

function with two quadratic polynomials and the single knot at  $v = k$  is defined as follows:

$$h = \beta_0 + \beta_1 v + \beta_2 v^2 + \beta_3 (v - k)^+ + \beta_4 [(v - k)^+]^2 \quad (4.1)$$

This spline function is illustrated below using the processing tank calibration data of September 1989 as listed in Table A-1 of Appendix A.

A review of the diagnostic plots (see Figures 2.1 and 2.2) indicates a change in the cross-sectional area of the tank at about ninety five liters; hence, the knot is assumed to be at that point. The model now becomes:

$$h = \beta_0 + \beta_1 v + \beta_2 v^2 + \beta_3 v_k + \beta_4 v_k^2 \quad (4.2)$$

where

$$v_k = \text{maximum value of } (v - 95, 0)$$

For this model, parameter estimates are obtained by using a "linear" least squares regression procedure in computer software provided by Statistical Analysis Software Inc. (SAS). The term "linear" here, applies to the normal equations in the regression analysis. The spline regression results are shown in Table 4.1.

TABLE 4.1

## Linear Least Squares Regression Results

## Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Value	Prob>F
Model	4	67958.04	16989.51	57985.58	0.0001
Error	16	4.69	0.29		
C Total	20	67962.73			

Root MSE	0.54129	R-square	0.9999
Dep Mean	160.13095	Adj R-sq	0.9999
C.V.	0.33803		

## Parameter Estimates

Var	DF	Parameter Estimate	Standard Error	T for H0: Parameter=0	Prob> T
b <sub>0</sub>	1	26.28729	1.4067390	18.687	0.0001
b <sub>1</sub>	1	0.92693	0.0489235	18.947	0.0001
b <sub>2</sub>	1	0.00076	0.0003828	1.996	0.0633
b <sub>3</sub>	1	-0.44011	0.0300605	-14.641	0.0001
b <sub>4</sub>	1	-0.00088	0.0003746	-2.357	0.0315

With the use of the linear regression parameter estimates, one can attempt to further enhance the model by assuming the location of the knot is unknown and using a "nonlinear" least squares modeling method. The term "nonlinear" here, again refers to the normal equations. When the position of the knot is not known, the solution to the normal equations can not be solved in closed form. For this reason, preliminary estimates of the model parameters must be known. Since the model with the knot at ninety five liters fit rather well, the estimates from this model can be used as the initial values.

The "nonlinear" regression procedure provided by SAS determines the optimal least squares parameter estimates with an iterative process. This method first takes combinations of preliminary parameter estimates in the neighborhood of the values specified and computes residual sums of squares. From this, an initial grid location to start the search is obtained. Next a multivariate secant iterative method is used to converge on the best estimate of the parameters. The convergence criteria is based on minimizing the residual sum of squares.

As seen in Table 4.2, the parameter estimates produced by this procedure are, indeed, quite similar to those obtained when the knot was assumed to be ninety five liters.

TABLE 4.2

## Nonlinear Least Squares Summary Statistics

Source	DF	Sum of Squares	Mean Square
Regression	5	606439.42	121287.88
Residual	16	3.67	0.23
Uncorrected Total	21	606443.09	
(Corrected Total)	20	67962.73	

## Parameter Estimates

$b_0$	26.60966610
$b_1$	0.91459941
$b_2$	0.00092688
$b_3$	-0.44700315
$b_4$	-0.00107033
KNOT	92.74615073



To obtain all of the regression summary statistics as given in Table 4.1, the "linear" least squares procedure is rerun with the new value of the knot being the estimate obtained by the "nonlinear" least squares procedure. These results are shown in Table 4.4.

By using these optimal least squares estimates of the parameters, the calibration function can be written as

$$\begin{aligned}
 H_{h(\text{new})} = & 27.241418 + 0.879996V + 0.001251V^2 \\
 & - 0.476178(V - 92.746)^+ \\
 & - 0.001382[(V - 92.746)^+]^2
 \end{aligned} \tag{4.3}$$

This function may be simplified by splitting it into two separate functions based on the value of V and the position of the knot. The simplified calibration function is shown in Table 4.3.

TABLE 4.3 Calibration Function  
Calibration Data of September 1989

Calibrated Volume (V in liters)	Liquid Height (H in cm)
$24.405 \leq V \leq 92.746$	$H = 27.2414 + 0.879996V + 0.001251V^2$
$92.746 < V \leq 320.025$	$H = 59.5173 + 0.660168V - 0.000131V^2$

TABLE 4.4

## Revised Linear Least Squares Regression Results

## Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Value	Prob>F
Model	4	67959.37	16989.84	81027.05	0.0001
Error	16	3.35	0.21		
C Total	20	67962.73			

Root MSE	0.45791	R-square	1.0000
Dep Mean	160.13095	Adj R-sq	0.9999
C.V.	0.28596		

## Parameter Estimates

Var	DF	Parameter Estimate	Standard Error	T for H0: Parameter=0	Prob> T
b <sub>0</sub>	1	27.24303	1.2207870	22.316	0.0001
b <sub>1</sub>	1	0.87991	0.0432785	20.331	0.0001
b <sub>2</sub>	1	0.00125	0.0003495	3.619	0.0023
b <sub>3</sub>	1	-0.47624	0.0261974	-18.179	0.0001
b <sub>4</sub>	1	-0.001383	0.0003391	-4.078	0.0009

**CHAPTER 5**  
**RECALIBRATIONS AND HISTORICAL DATA**

All processing tanks need to be recalibrated on a routine schedule because of the difficulties in assuring a stable system over extended periods of time. This is especially true for the ring-filled processing tanks whose internal structure is subject to ever changing conditions. Several factors which may lead to this change include the addition or removal of rings, the breaking and/or compaction of the rings, or the build up of sludge precipitating out of the solution in the tank. If the calibration relationship changes or shifts, it is important to treat the calibration data in an appropriate way to determine the best estimates of the calibration model parameters and the uncertainties in the calculated volumes.

The first recalibration of a processing tank will provide a new data set to be modeled. This new calibration model then needs to be compared to the original calibration model to examine their similarities and differences. Assuming the error term variances in the regression models for the different calibration data sets are approximately equal, the use of the general linear test and indicator variables permits one to test the equality of the different calibration functions.

The general linear test can be described as follows. For the simple linear regression case, a full model is:

$$y_i = \beta_0 + \beta_1 X_i + \epsilon_i . \quad (5.1)$$

This model is fit by the method of least squares and an error sum of squares (SSE) is obtained. This sum of squares will be called  $SSE(F)$  to indicate that it measures the variation of  $y_i$  around the regression line for the full model.

Next, consider a reduced or restricted model:

$$y_i = \beta_0 + \epsilon_i . \quad (5.2)$$

This model exists when the null hypothesis

$$H_0: \beta_1 = 0$$

is true. The reduced model is also fit by the method of least squares and an error sum of squares is obtained which is denoted by  $SSE(R)$ .

The logic now is to compare  $SSE(F)$  and  $SSE(R)$ . It can be shown that  $SSE(F)$  is never greater than  $SSE(R)$ . The reason is that the more parameters used in the model, the

better one can fit the data and the deviations become smaller. If the full model does not reduce the variability by much more than the reduced model, then the data suggests  $H_0$  holds. This means that the variation of the observations around the regression for the full model is almost as great as that around the regression for the reduced model.

The actual test statistic used is a function of  $SSE(R) - SSE(F)$ , namely:

$$F^* = \frac{SSE(R) - SSE(F)}{df_R - df_F} + \frac{SSE(F)}{df_F} \quad (5.3)$$

which follows the F distribution if  $H_0$  and the other "normal error" assumptions hold. The degrees of freedom  $df_R$  and  $df_F$  are those associated with the reduced and full model error sum of squares, respectively. (Neter, Wasserman, and Kutner 1985).

This general linear test approach can be used to determine if calibration models for a specific tank change over time. To use this test, the full model would be determined by fitting separate regression functions to the recalibration data and the historical calibration data. The reduced model would be determined by fitting one regression function to the combined data for all of the calibration

runs. If the general linear test shows the full model to be significantly different than the reduced model, then the processing tank has changed. That is, the previous calibration model and data are no longer representative of the current conditions in processing tank. The correct calibration model now becomes the one derived from the recalibration data.

For an example, consider the ring-filled processing tank data as shown in Table A-1 of Appendix A. In November of 1985, two calibration runs were made on a clean processing tank before it went into production. In January of 1986, a recalibration run was made as part of the routine schedule. Unfortunately, only one run was made at this time because more runs would lead to a longer down time and generate more hazardous wastes.

The analysis and modeling of the data from the two calibration runs made in November of 1985 led to a spline model consisting of two quadratic polynomials as follows

$$H = \beta_0 + \beta_1 V + \beta_2 V^2 + \beta_3 V_j + \beta_4 V_j^2 \quad (5.4)$$

where

$$V_j = \text{maximum value of } (V - 165.34, 0) .$$

The optimal least square estimates obtained from SAS are as follows

$$\begin{array}{ll} b_0 = 17.426966 & b_3 = -0.065422 \\ b_1 = 1.016619 & b_4 = 0.000779 \\ b_2 = -0.000949 & SSE = 4.46592 \end{array}$$

The analysis and modeling of the data from the single calibration run made in January of 1986 also led to a spline model consisting of two quadratic polynomials as follows

$$H = \beta_0 + \beta_1 V + \beta_2 V^2 + \beta_3 V_1 + \beta_4 V_1^2 \quad (5.6)$$

where

$$V_1 = \text{maximum value of } (V - 144.92, 0).$$

The optimal least square estimates obtained from SAS are as follows:

$$\begin{array}{ll} b_0 = 21.003535 & b_3 = -0.112241 \\ b_1 = 1.034378 & b_4 = 0.000922 \\ b_2 = -0.001032 & SSE = 0.79604 \end{array}$$

With the use of indicator variables, a full model which fits separate regression lines to the data from each population can be written as

$$\begin{aligned}
 H = & \beta_0 + \beta_1 V + \beta_2 V^2 + \beta_3 V_j (1-x) + \beta_4 V_j^2 (1-x) + \beta_5 x + \beta_6 Vx \\
 & + \beta_7 V^2 x + \beta_8 V_1 x + \beta_9 V_1^2 x \quad (5.6)
 \end{aligned}$$

where

$$\begin{aligned}
 V_j &= \text{maximum value of } (V - 165.34, 0) && \text{November 1985} \\
 V_1 &= \text{maximum value of } (V - 144.92, 0) && \text{January 1986} \\
 x &= 0 \text{ for November 1985 data and} \\
 x &= 1 \text{ for January 1986 data.}
 \end{aligned}$$

When  $x = 0$ , the full model equation reduces to

$$H = \beta_0 + \beta_1 V + \beta_2 V^2 + \beta_3 V_j + \beta_4 V_j^2, \quad (5.7)$$

and when  $x = 1$ , the full model reduces to

$$H = (\beta_0 + \beta_5) + (\beta_2 + \beta_6) V + (\beta_3 + \beta_7) V^2 + \beta_8 V_1 + \beta_9 V_1^2 \quad (5.8)$$



These equations are in the same form as those for the calibration models determined earlier for these two sets of data. (see eq [5.4] and [5.5])

The parameter estimates of the full model as obtained by the method of linear and non-linear least squares from SAS are as follows:

$$\begin{array}{ll} b_0 = 17.427 & b_5 = 3.576 \\ b_1 = 1.017 & b_6 = 0.017758 \\ b_2 = -0.000949 & b_7 = -0.000083 \\ b_3 = -0.065422 & b_8 = -0.112241 \\ b_4 = 0.000779 & b_9 = 0.000922 \end{array}$$

The associated error sum of squares and degrees of freedom for the full model as obtained from SAS are

$$\text{SSE}(F) = 5.26 \quad \text{df}_f = 56.$$

Note that the  $\text{SSE}(F)$  is equivalent to the sum of the SSE's for the two separate models.

The reduced model for the combined calibration data from all three runs is also a spline model with two quadratic polynomials as follows

$$H = \beta_0 + \beta_1 V + \beta_3 V^2 + \beta_4 V_m + \beta_5 V_m^2 \quad (5.9)$$

where

$$V_m = \text{maximum value of } (V - 160.32, 0) .$$

The associated error sum of squares and degrees of freedom for the reduced model as obtained from SAS are

$$\text{SSE(R)} = 128.89 \quad \text{df}_R = 61.$$

Now, to compare the full model to the reduced model, the general linear test is used. The associated null and alternative hypotheses are

$H_0$ : Reduced model is sufficient

$H_a$ : Full model is sufficient.

The associated  $F^*$  statistic (see eq. [5.3]) is

$$F^* = \frac{128.89 - 5.26}{61 - 56} + \frac{5.26}{56} = 263.24$$

The critical value for  $\alpha = 0.05$  is

$$F(0.95, 5, 56) \approx 2.4$$

Since the calculated  $F^*$  statistic is greater than the associated critical value, the null hypothesis is rejected and the alternative hypothesis is accepted. That is, the full model which uses separate calibration functions to model the November 1985 data and the January 1986 data, becomes the accepted model. This shows that the variation of the observations around the full regression model is significantly less than the variation around the reduced model. In other words, the internal structure of the processing tank has changed over time and the previous calibration function is no longer representative of the current conditions of the tank. The recalibration data collected in January 1986 should be modeled independently of the historical data to provide the most accurate model of the tank.

If the full model did not significantly reduce the variation of the observations about the regression function, then the accepted model would be the reduced model. This model would fit a single calibration function to all of the calibration data.

When the tank is next recalibrated, the new data should only be compared to the original calibration data. This

will help determine when the tank has changed enough for the calibration model to be significantly different than the original tank calibration model. The recalibration data collected in between is not used for the following reason.

Suppose the first recalibration model is not significantly different than the original model. The correct model would then be determined by combining all of the data. If the next recalibration model was compared to this new model, it may not be significantly different, but it may be significantly different than the original data. If the new recalibration model is different than the original model, then the tank has changed and a new model is necessary to accurately model the tank. By making the comparison to the original model, a slow drift of the calibration function over time can be detected. This allows for a new model to be developed when the data suggests that the interior of the tank has undergone significant changes.

**CHAPTER 6**  
**VOLUME CALCULATION**

To obtain a volume estimate, the calibration function is used to make a prediction of the volume which gave rise to a new observation of liquid height in the sight gauge. This process is known as inverse prediction. To obtain the volume calculation function, the estimated calibration function must be inverted.

In inverse prediction for a simple linear model, an estimated calibration function based on  $n$  observations is

$$H = b_0 + b_1V . \quad (6.1)$$

When a new observation  $H_{h(new)}$  becomes available, it is desirable to estimate the value of  $V_{h(new)}$  which gave rise to this variable. A point estimator is obtained by solving equation 6.1 for  $V$ , given  $H_{h(new)}$

$$V_{h(new)} = \frac{H_{h(new)} - b_0}{b_1} \quad b_1 \neq 0$$

Similarly, for a simple quadratic model, an estimated calibration function based on  $n$  observations is

$$H = b_0 + b_1V + b_2V^2 . \quad (6.2)$$

For a new observation  $H_{h(new)}$ , a point estimator of  $V_{h(new)}$  is obtained by solving equation 6.2 for  $V$ , given  $H_{h(new)}$

$$V_{h(new)} = \frac{-b_1 \pm \sqrt{b_1^2 - 4b_2(b_0 - H_{h(new)})}}{2b_2} \quad b_2 \neq 0$$

For example, the calibration function as shown in Table 4.3, is inverted and the results are shown in Table 6.1. This table can then be used to calculate volume estimates for a given observation of  $H$ .

TABLE 6.1 Volume Function

Calibration Data of September 1989

Liquid Height (H in cm)	Calibrated Volume (V in liters)
$49.70 \leq H \leq 119.62$	$V = -351.717$ $+ (0.63808 + 0.005004H)^{1/2}/0.002502$
$119.62 < H \leq 257.45$	$V = 2519.725$ $+ (0.46701 - 0.000524H)^{1/2}/-0.000262$

**CHAPTER 7**  
**VOLUME UNCERTAINTIES**

Providing estimates of calculated volume uncertainty is an integral part of the calibration process and one of the most difficult. When a new observation of height,  $H_{h(\text{new})}$ , becomes available, an estimate of the volume contained in the tank can be obtained. It is also desirable to be able to calculate a prediction interval about this volume estimate. An accepted method to determine the prediction intervals associated with volume measurements is illustrated for a simple linear regression model.

As shown in Figure 7.1, the fitted straight line and the curves that give the end points of the  $100(1-\alpha)\%$  prediction intervals for new values of  $H$ , for a given  $V$ , are drawn. For inverse prediction, a new observation  $H_{h(\text{new})}$  is obtained and a horizontal line is drawn parallel to the  $V$ -axis at this value. Where this straight line cuts the prediction limits, perpendicular lines are drawn down to the  $V$ -axis. This gives the lower and upper  $100(1-\alpha)\%$  "fiducial limits" for the estimated volume as labeled in Figure 7.1 as  $V_l$  and  $V_u$ . For well determined regression lines, these limits may be simply regarded as the inverse prediction limits for volume estimates. (Draper, Smith 1981)

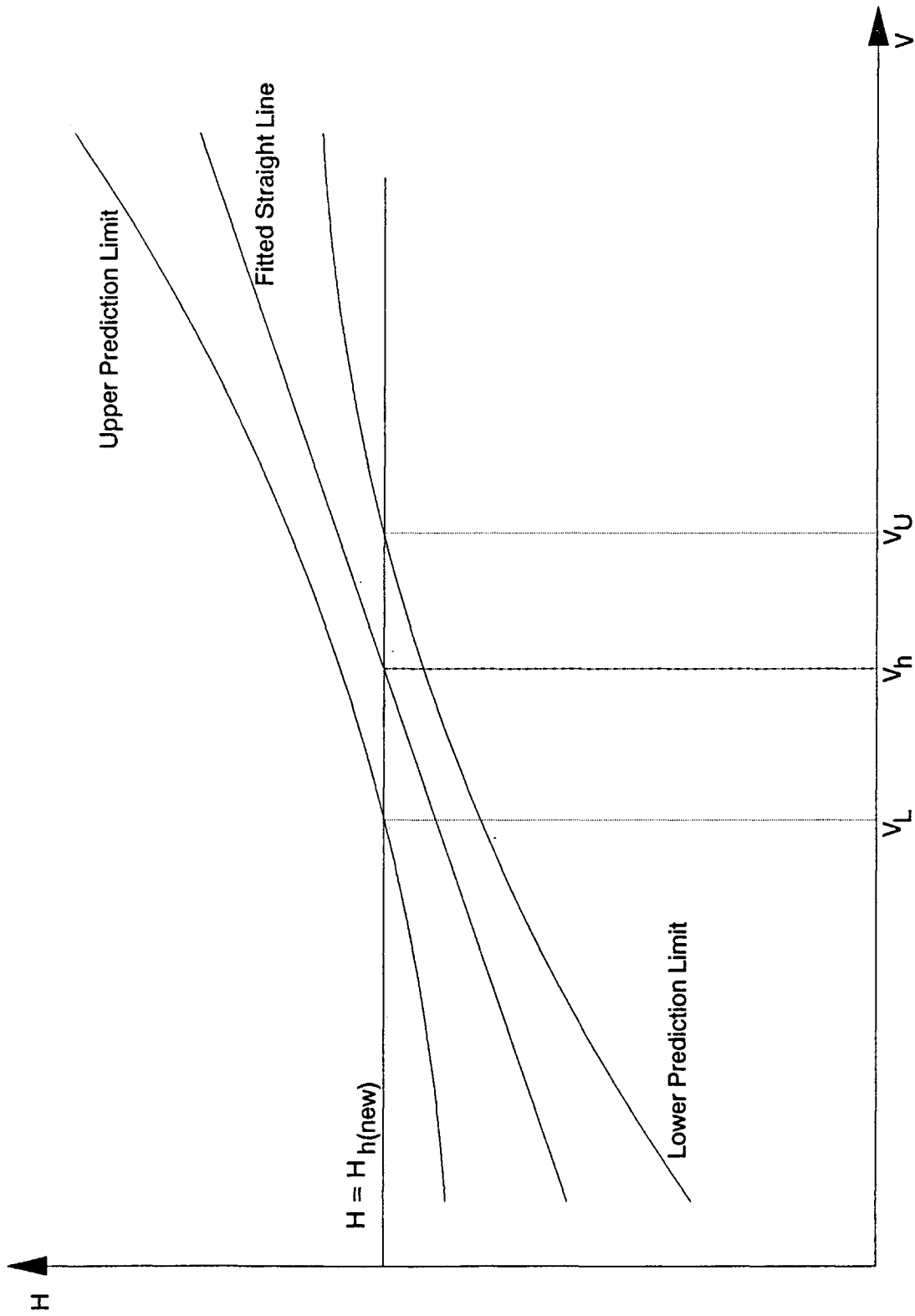


FIGURE 7.1 Inverse Prediction



When the regression line is not well determined, peculiarities may arise. The lines that give the end points of  $100(1-\alpha)\%$  prediction intervals will be wider apart and they may flare out badly. This may lead to values of  $V_L$  and  $V_U$  that are both on one side of the estimated volume. Another possibility is that the values of  $V_L$  and  $V_U$  cannot be determined because the horizontal line at  $H_{h(\text{new})}$  never intersects the prediction limit lines. Figure 7.2 shows examples of these possibilities.

To obtain the prediction intervals for volume measurements, the prediction limits for liquid height measurements must be inverted. This inversion is very difficult when using spline models due to the complexity of the equations. The general form of the equation for  $100(1-\alpha)\%$  prediction limits for a new observation is

$$H_{h(\text{new})} \pm t(1 - \alpha/2; n - p)s(H_{h(\text{new})}) \quad (7.1)$$

where

$H_{h(\text{new})}$  = height calculated from the calibration function  
given  $V_{h(\text{new})}$

$\alpha$  = probability of a type I error

$n$  = number of data points in the calibration model

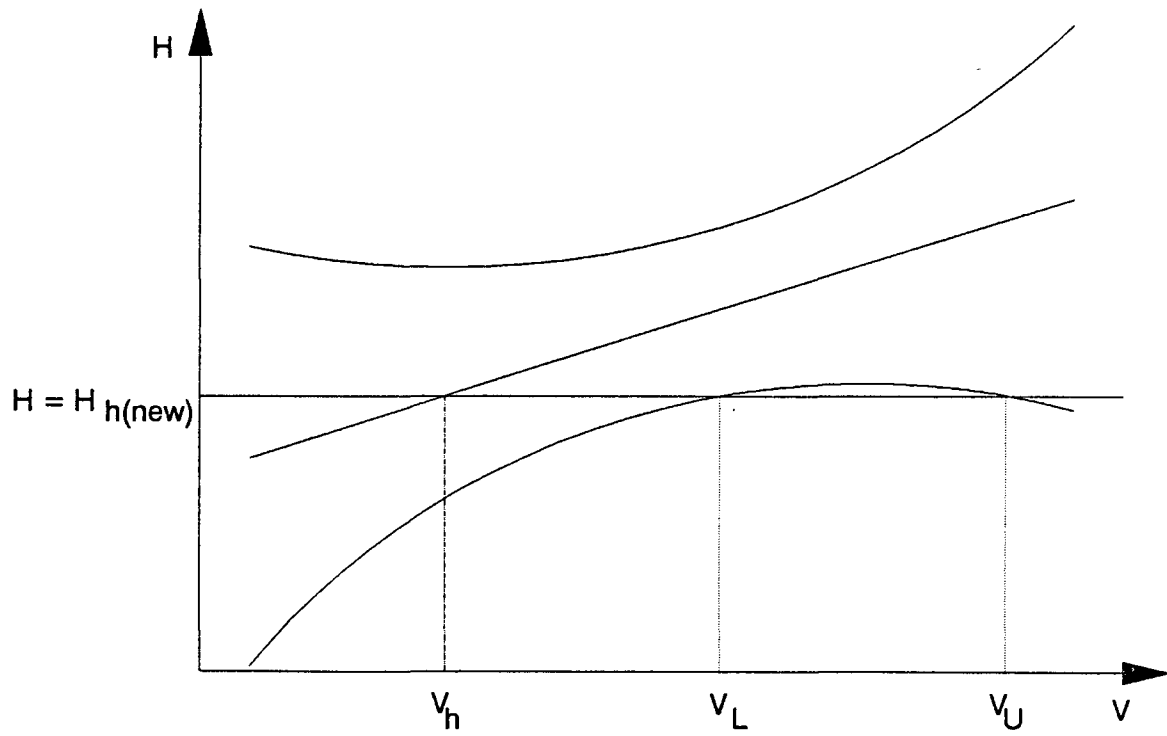
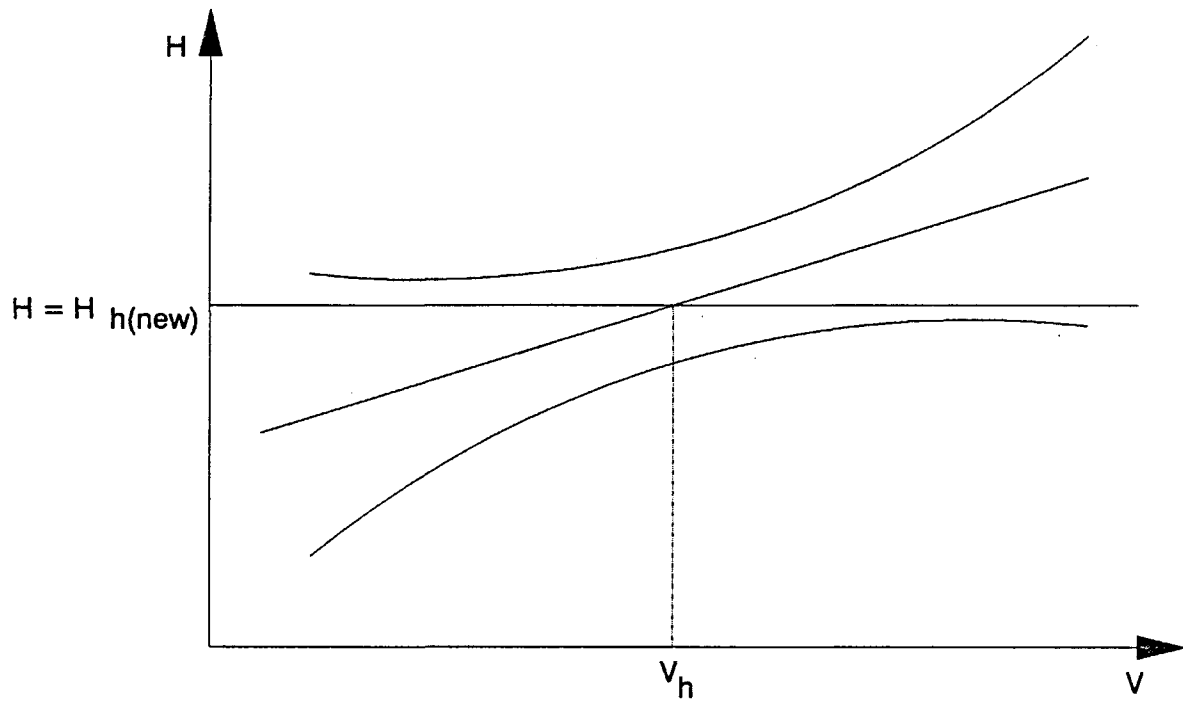


FIGURE 7.2 Inverse Prediction Peculiarities

$p$  = number of parameters being estimated in the model

and

$s^2(H_{h(\text{new})})$  = the estimated variance of  $H_{h(\text{new})}$

With the use of matrix notation and summary statistics, the estimated variance of  $H_{h(\text{new})}$  may be determined from

$$s^2(H_{h(\text{new})}) = MSE(1 + W_h'(W'W)^{-1}W_h) \quad (7.2)$$

where

$W$  = a matrix containing a column of ones and columns containing the independent variables

$W_h$  = a column vector for any new observation  $V_{h(\text{new})}$

and

$MSE$  = the error or residual mean square

For a new observation  $H_{h(\text{new})}$ , the values of  $V_L$  and  $V_U$  can be obtained as follows. In figure 7.1,  $V_L$  is the V-coordinate of the point of intersection of the horizontal line

$$H = H_{h(\text{new})} \quad (7.3)$$

and the curve

$$H = H_{V_L} + tS(H_{h(new)}) \quad (7.4)$$

where

$H_{V_L}$  = the calibration function as shown in Table 4.3.

Setting equations 7.3 and 7.4 equal to each other gives

$$H_{h(new)} = H_{V_L} + tS(H_{h(new)}) \quad (7.5)$$

which can be expanded by using equation 7.2 to give

$$H_{h(new)} = H_{V_L} + t\sqrt{MSE(1 + W'_{V_L}(W/W)^{-1}W_{V_L})}$$

Thus, the lower 100(1- $\alpha$ )% prediction limit for V can be obtained by solving the above equation for  $V_L$ . Similarly, the upper 100(1- $\alpha$ )% prediction limit for V can be obtained by solving the following equation for  $V_U$

$$H_{h(new)} = H_{V_U} - t\sqrt{MSE(1 + W'_{V_U}(W/W)^{-1}W_{V_U})}$$

For spline calibration models, the equations 7.6 and 7.7 are not easily inverted for calculating the prediction limits  $V_L$  and  $V_U$  for  $V$ . However, a computer program can be utilized to obtain accurate values for  $V_L$  and  $V_U$ .

For an example of calculating volume uncertainties, once again consider the calibration data obtained in September 1989 as shown in Table A-1 of Appendix A. By substituting the calibration function (see eq. [4.3]) for  $V_L$  into equation 7.6, the following equation is obtained

$$\begin{aligned}
 H_{h(new)} = & 27.241418 + 0.879996V_L + 0.001251V_L^2 \\
 & - 0.476178(V_L - 92.746) - 0.001382((V_L - 92.746)^+)^2 \\
 & + t\sqrt{MSE(1 + W_{V_L}'(W'W)^{-1}W_{V_L})} \qquad (7.8)
 \end{aligned}$$

To solve equation 7.8 for  $V_L$ , given  $H_{h(new)}$ , the numerical method of bisection can be used. This method will repeatedly generate approximate values,  $V_L$ , until it finds a  $V_L$  approximation that is certain to be within a distance epsilon from the true value. A computer program written in Fortran utilizes the bisection method to calculate approximate values of  $V_L$  and  $V_U$ . (see Appendix B)

For a  $H_{h(\text{new})} = 100.0$  cm, the following estimates may be obtained

$$V_{h(\text{new})} = 74.74 \text{ liters}$$

$$V_L = 73.71 \text{ liters and}$$

$$V_U = 75.76 \text{ liters.}$$

The prediction interval in this example provides bounds of approximately  $\pm 1.4\%$  of the estimated volume. Additional volume estimates and prediction intervals are found in Table 8.2.

**CHAPTER 8**  
**COMPARISON TO LINEAR MODEL**

A common technique used in industry today is to assume that processing tanks have a constant cross-sectional area and thus the calibration model is the simple linear model

$$H = b_0 + b_1V . \quad (8.1)$$

By inverting this calibration model, the volume calculation function is simply

$$\hat{V} = \frac{H_{h(new)} - b_0}{b_1} \quad b_1 \neq 0 \quad (8.2)$$

Although this technique is easy to use, it does not always provide accurate calibration results. This is especially true when the processing tank being modeled has a varying internal structure like the ring-filled tanks. To accurately model the calibration data, comparisons need to be made among the different modeling techniques. This section will provide comparisons of a linear model and a spline model (see eq. [4.3]) for the tank calibration data collected in September of 1989 (see Appendix A).

Before any comparison can be made, the least squares regression statistics must be obtained for the linear model. The results obtained from SAS are shown in Table 8.1. Equation 8.2 may now be rewritten as

$$H = 49.726884 + 0.671835V \quad (8.3)$$

The simplest comparison to make is to graphically compare the residuals from each model. The residual is calculated by taking the predicted value of height and subtracting the actual value. The residuals are then plotted against volume as shown in Figure 8.1. A review of this plot clearly shows that the spline model gives a better fit to the data. Another method of comparison is to look at the adjusted R-squared values for both models.

The coefficient of multiple determination, denoted by  $R^2$ , is defined as follows

$$R^2 = 1 - \frac{SSE}{SSTO}$$

where

SSE = error sum of squares and

SSTO = total sum of squares.



TABLE 8.1  
 Linear Least Squares Regression Results  
 Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Value	Prob>F
Model	1	67148.02	67148.02	1565.98	0.0001
Error	19	814.70	42.88		
C Total	20	67962.73			

Root MSE	6.54822	R-square	0.9880
Dep Mean	160.13095	Adj R-sq	0.9874
C.V.	4.08929		

Parameter Estimates

Var	DF	Parameter Estimate	Standard Error	T for H0: Parameter=0	Prob> T
$b_0$	1	49.726884	3.1345689	15.864	0.0001
$b_1$	1	0.671835	0.0169773	39.572	0.0001

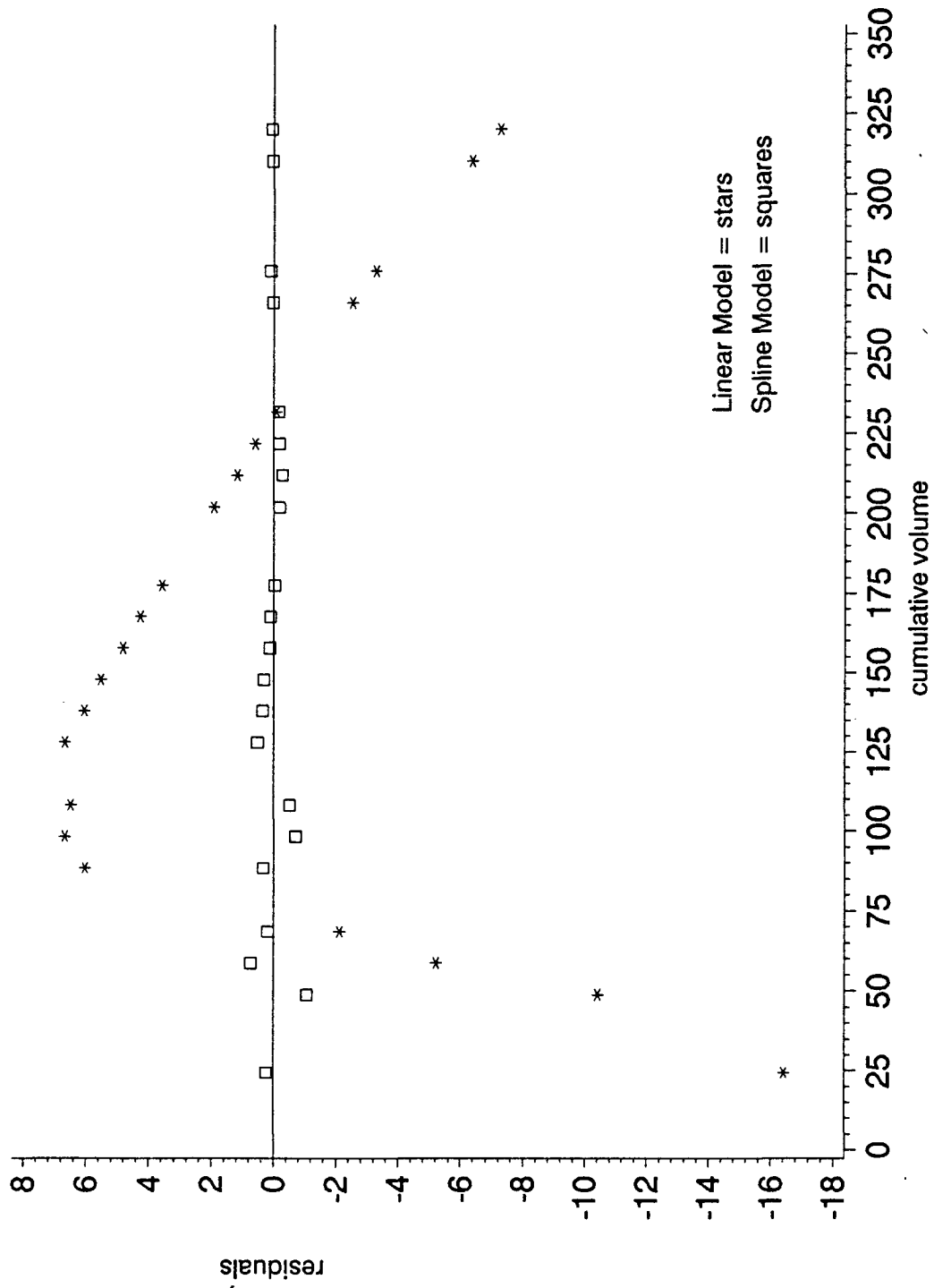


FIGURE 8.1 Linear Model and Spline Model Residuals

Calibration data from September 1989

This value measures the proportionate reduction of total variation in height measured (H) associated with the use of the set of volume (V) variables. Since  $R^2$  often can be made large by including a large number of independent variables, it is suggested that a modified measure be used which recognizes the number of independent variables in the model. The adjusted coefficient of multiple determination, denoted by  $R_a^2$ , is defined:

$$R_a^2 = 1 - \frac{(n - 1)}{(n - p)} \frac{SSE}{SSTO}$$

where

n = number of data points being modeled and

p = number of parameters being estimated

This adjusted coefficient may actually become smaller when another independent variable is introduced into the model, because the decrease in SSE may be more than offset by the loss of a degree of freedom in the denominator, n-p. (Neter, Wasserman, and Kutner 1985)

From Tables 8.1 and 4.4, the adjusted R-squared values are found to be

Spline Model  $R_a^2 = 0.9999$

Linear Model  $R_a^2 = 0.9874$

Although these large values would suggest that both models fit the data rather well, a large  $R_a^2$  does not necessarily imply that the fitted model is a useful one.

The usefulness of a regression relation depends upon the width of the prediction interval and the particular needs for precision, which vary from one application to another. Hence, no single measure is an adequate indicator of the usefulness of the regression relation. (Neter, Wasserman, and Kutner 1985) One important statistic used in calculating a prediction interval (see equations [7.1] and [7.2]) is the error mean square or residual mean square (MSE). The MSE is an unbiased estimator of the variance of the error terms in a regression model which can be defined as

$$MSE = \frac{SSE}{n - p} = \frac{\sum (H_i - H_{est})^2}{n - p}$$

where

$n$  = number of data points being modeled

$p$  = number of parameters being estimated

$H_i$  = actual value of height in the sight gauge and  
 $H_{est}$  = estimated value of height.

The smaller the value of MSE, the less the variance of the error terms for the model. From Tables 8.1 and 4.4, the MSE values for the two models are found to be

Spline Model MSE = 0.21

Linear Model MSE = 42.88

This comparison again suggests that the spline model provides a better representation of the calibration data than does the linear model.

Finally, some sample calculations are made to determine volume estimates and prediction intervals, from both models, for given values of  $H_{h(new)}$ . The equations necessary to calculate these values from the spline model have been discussed in great detail in previous chapters. For the linear model, the volume estimate may be obtained by inverting equation 8.3 which gives

$$\hat{V}_{h(new)} = \frac{H_{h(new)} - 49.726884}{0.671835V} \quad (8.4)$$

Also, for inverse prediction of a linear model, the approximate  $100(1 - \alpha)\%$  prediction intervals are

$$\hat{V}_{h(new)} \pm t(1 - \alpha/2; n - 2) S(\hat{V}_{h(new)}) \quad (8.5)$$

where

$$S^2(\hat{V}_{h(new)}) = \frac{MSE}{b_1^2} \left[ 1 + \frac{1}{n} + \frac{(\hat{V}_{h(new)} - \bar{V})^2}{\sum (V_i - \bar{V})^2} \right]$$

Table 8.2 provides the volume estimates and prediction intervals from both models for several values of  $H_{h(new)}$ .

The results in Table 8.2 show drastic differences between the two types of models. Not only do the estimated volumes differ, but the prediction intervals from the linear model are almost an order of magnitude larger than those from the spline model. This is mainly due to the large difference in the MSE's for the two models.

TABLE 8.2  
Comparison of Spline and Linear Models

Height (cm)	<u>SPLINE MODEL</u>		<u>LINEAR MODEL</u>	
	Vol. Est. (liters)	95% Pred. Int. (liters)	Vol. Est. (liters)	95% Pred. Int. (liters)
75.0	50.63	(49.51, 51.75)	37.62	(16.21, 59.03)
100.0	74.74	(73.71, 75.76)	74.83	(53.67, 95.99)
125.0	101.22	(99.48, 102.95)	112.04	(91.06, 133.02)
150.0	141.00	(139.36, 142.65)	149.25	(128.36, 170.15)
175.0	181.46	(179.73, 183.19)	186.46	(165.58, 207.35)
200.0	222.63	(220.77, 224.48)	223.68	(202.71, 244.64)
225.0	264.56	(262.50, 266.59)	260.89	(239.76, 282.01)
250.0	307.27	(304.83, 309.73)	298.10	(276.73, 319.38)

**CHAPTER 9**  
**CONCLUSIONS AND RECOMMENDATIONS**

The intent of the calibration procedure for processing tanks is to determine an accurate relationship between the liquid measurement response and the volume content of the tank. Once this relationship is determined, estimated volumes and their associated prediction intervals may be inversely predicted from new values of the liquid response measurement. For the ring-filled processing tank examined in this paper, several conclusions can be made.

1) A spline function should be used to provide an accurate calibration model. The processing tank needs to be modeled in segments because it does not have a constant cross-sectional area. Diagnostic plots such as profile plots and incremental slope plots may be helpful in determining the joints of these segments.

2) A statistical test needs to be made to determine if recalibration data is significantly different from historical data before the historical data can be included in the new model. The internal structure of the ring-filled tank may change as the rings shift, break, and/or compact. If the internal structure of the tank changes, then the



historical data is no longer representative of the current conditions. The calibration model must change as the tank changes.

3) The spline model provides more accurate volume estimates and much tighter prediction intervals than a linear model does. This is mainly attributed to the fact that the error mean square (MSE) for the spline model is much less than that of the linear model.

Although the spline model provided a more accurate calibration model for the processing tank examined, it may not be as useful for other processing tanks. The simple linear calibration model makes the calculations much easier and it may provide the accuracy needed. It is important that the calibration data from processing tanks be examined on an individual basis and the appropriate calibration model be determined.

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**APPENDIX A**  
**TANK CALIBRATION DATA**

TABLE 1  
Ring-Filled Tank Calibration Data

<u>November 1985</u>		<u>November 1985</u>		<u>January 1986</u>		<u>August 1986</u>	
V(l)	H(cm)	V(l)	H(cm)	V(l)	H(cm)	V(l)	H(cm)
48.836	64.98	48.836	64.30	68.624	87.08	48.818	70.70
68.624	82.80	68.624	82.79	78.518	95.78	58.738	80.30
78.518	91.30	78.518	91.43	98.306	113.14	68.658	90.20
88.412	100.08	88.412	100.20	108.200	120.92	78.578	100.18
98.306	108.55	98.306	108.80	118.094	128.22	88.498	109.80
108.200	115.90	108.200	116.42	137.882	144.19	98.418	118.49
118.094	123.84	118.094	124.32	147.776	151.04	108.338	126.22
127.988	131.15	127.988	131.58	157.670	157.28	128.178	140.30
137.882	139.25	137.882	139.93	167.564	163.41	138.098	146.60
147.776	146.75	147.776	147.35	177.458	169.35	148.018	152.65
157.670	154.18	157.670	154.82	187.352	175.28	157.938	158.84
167.564	161.00	167.564	161.12	211.770	190.04	167.858	164.79
177.458	167.37	177.458	167.45	221.664	196.43	177.778	170.60
187.352	173.35	187.352	173.45	231.558	202.50	187.698	176.52
211.770	188.20	211.770	188.49	255.976	217.15	212.107	191.38
221.664	194.42	221.664	194.78	265.870	223.14	222.027	197.60
231.558	200.98	231.558	201.38	275.764	229.00	231.947	203.48
255.976	216.25	255.976	216.10	285.658	234.80	256.356	218.10
265.870	222.27	265.870	222.10	310.076	249.05	266.276	224.00
275.764	228.09	275.764	228.00	319.970	254.85	276.196	229.82
285.658	233.90	285.658	233.85			286.116	235.82
310.076	248.13	310.076	248.08			310.525	250.00
319.970	254.03	319.970	253.92			320.445	255.71
						330.365	261.50

TABLE 1 (continued)

<u>August 1987</u>		<u>August 1988</u>		<u>September 1989</u>	
V(l)	H(cm)	V(l)	H(cm)	V(l)	H(cm)
48.818	71.14	48.818	70.55	24.405	49.70
58.738	81.95	58.738	81.10	48.810	72.10
68.658	92.45	68.658	91.45	58.710	83.95
78.578	103.19	78.578	101.60	68.610	93.70
88.498	113.45	88.498	111.65	88.410	115.15
98.418	121.67	98.418	120.35	98.310	122.45
108.338	128.25	108.338	126.72	108.210	128.90
128.178	141.50	128.178	140.07	128.010	142.40
138.098	147.51	138.098	146.20	137.910	148.42
148.018	153.78	148.018	152.15	147.810	154.55
157.938	159.88	157.938	158.30	157.710	160.50
167.858	165.74	167.858	164.35	167.610	166.60
177.778	171.72	177.778	170.30	177.510	172.55
202.187	186.30	202.187	184.75	201.915	187.30
212.107	192.40	212.107	190.90	211.815	193.20
222.027	198.40	222.027	196.90	221.715	199.28
231.947	204.20	231.947	202.72	231.615	205.25
256.356	218.90	256.356	217.42	265.920	225.85
266.276	224.80	266.276	223.30	275.820	231.75
276.196	230.52	276.196	229.25	310.125	251.70
286.116	236.35	286.116	235.05	320.025	257.45
310.525	250.21	310.525	249.40		
320.445	256.50	320.445	255.00		
330.365	262.20				

**APPENDIX B**  
**COMPUTER PROGRAM**

```
* VOLUME AND UNCERTAINTY CALCULATIONS
* TANK 1022 CALIBRATION DATA 9/89
* JOHN F. BAUER III
*
```

```
* VARIABLE DECLARATION
*
```

```
IMPLICIT NONE
INTEGER I,J
REAL X(5), XPXI(5,5),TEMP(5), YNEW, DIF, DUMMY
REAL B0,B1,B2,B3,B4,K,T,MSE,YH,XH,LO,HIGH,C,MID,XK,FX1,FX2
```

```
* VALUES OF THE X'X INVERSE MATRIX
*
```

```
XPXI(1,1)=7.107559152
XPXI(1,2)=-0.241675992
XPXI(1,3)=0.0018224999
XPXI(1,4)=-0.10288876
XPXI(1,5)=-0.001799283
XPXI(2,1)=XPXI(1,2)
XPXI(2,2)=0.0089327578
XPXI(2,3)=-0.000070405
XPXI(2,4)=0.0044576173
XPXI(2,5)=0.0000692244
XPXI(3,1)=XPXI(1,3)
XPXI(3,2)=XPXI(2,3)
XPXI(3,3)=0.0000005708
XPXI(3,4)=-0.000039026
XPXI(3,5)=-0.000000558
XPXI(4,1)=XPXI(1,4)
XPXI(4,2)=XPXI(2,4)
XPXI(4,3)=XPXI(3,4)
XPXI(4,4)=0.0032731032
XPXI(4,5)=0.0000371851
XPXI(5,1)=XPXI(1,5)
XPXI(5,2)=XPXI(2,5)
XPXI(5,3)=XPXI(3,5)
XPXI(5,4)=XPXI(4,5)
XPXI(5,5)=0.0000005483
```

```
* OPTIMAL LEAST SQUARES ESTIMATES
*
```

```
B0=27.243036658
B1=0.879915002
B2=0.0012518854
B3=-0.476236929
B4=-0.001382694
K=92.746
MSE=0.20968
```



```

*
*   ASSOCIATED T DISTRIBUTION VALUE
*
*   T=2.12
*
*   TAKE SIGHT GAUGE OBSERVATION AND CALCULATE ESTIMATED VOLUME
*
5  WRITE(5,*) 'INPUT THE SIGHT GAUGE READING IN CM'
   READ(5,*) YH
   WRITE(5,*) 'FOR A SIGHT GAUGE READING OF ',YH,' cm'
   IF ((YH .GE. 49.70) .AND. (YH .LE. 119.62)) THEN
     XH = -351.717 + SQRT(0.63808 + 0.005004*YH)/0.002502
   ELSE IF ((YH .GT. 119.62) .AND. (YH .LE. 257.45)) THEN
     XH = 2519.725 + SQRT(0.46701 - 0.000524*YH)/-0.000262
   ELSE
     WRITE(5,*) 'SIGHT GAUGE READING IS OUT OF RANGE FOR THE MODEL'
     GOTO 5
   ENDIF
   WRITE(5,*) 'THE ESTIMATED VOLUME = ',XH, 'LITERS'
*
*   CONSTANTS USED IN BISECTION METHOD
*
*   C=5
*   YNEW=1000
*   LO=XH
*   HIGH=XH+C
*
*   BISECTION METHOD FOR UPPER 95% PREDICTION LIMIT
*
DO WHILE (ABS(YH-YNEW) .GT. 0.001)
  MID=(LO+HIGH)/2.0
  XK=MAX(MID-K,0.0)
  FX1=B0+B1*MID+B2*MID**2+B3*XK+B4*XK**2
*
*   X VECTOR VALUES
*
  X(1)=1
  X(2)=MID
  X(3)=MID**2
  X(4)=XK
  X(5)=XK**2
*
*   PERFORM MATRIX MULTIPLICATION
*

```

```

DUMMY=0
DO 25 I=1,5
    TEMP(I)=0
    DO 15 J=1,5
        TEMP(I)=TEMP(I)+X(J)*XPXI(J,I)
15    CONTINUE
DUMMY=DUMMY+TEMP(I)*X(I)
25    CONTINUE
*
*    DETERMINE IF THE BISECTION METHOD HAS CONVERGED
*
FX2=T*SQRT(MSE*(1+DUMMY))
YNEW=FX1-FX2
IF ((YH-YNEW) .LT. 0) THEN
    HIGH=MID
ELSE
    LO=MID
END IF
END DO
*
*    OUTPUT UPPER 95% PREDICTION LIMIT
*
WRITE(5,*) 'the upper 95% prediction limit = ', MID, 'liters'
*
*    RE-INITIALIZE CONSTANTS FOR BISECTION METHOD
*
YNEW=1000.0
HIGH=XH
LO=XH-C
*
*    BISECTION METHOD FOR LOWER 95% PREDICTION LIMIT
*
DO WHILE (ABS(YH-YNEW) .GT. 0.0001)
    MID=(LO+HIGH)/2.0
    XK=MAX(MID-K,0.0)
    FX1=B0+B1*MID+B2*MID**2+B3*XK+B4*XK**2
*
*    X VECTOR VALUES
*
X(1)=1
X(2)=MID
X(3)=MID**2
X(4)=XK
X(5)=XK**2
*
*    PERFORM MATRIX MULTIPLICATION
*

```

```
DUMMY=0
DO 45 I=1,5
  TEMP(I)=0
  DO 35 J=1,5
    TEMP(I)=TEMP(I)+X(J)*XPXI(J,I)
35  CONTINUE
  DUMMY=DUMMY+TEMP(I)*X(I)
45  CONTINUE
*
*   DETERMINE IF THE BISECTION METHOD HAS CONVERGED
*
  FX2=T*SQRT(MSE*(1+DUMMY))
  YNEW=FX1+FX2
  IF ((YH-YNEW) .LT. 0) THEN
    HIGH=MID
  ELSE
    LO=MID
  END IF
END DO
*
*   OUTPUT LOWER 95% PREDICTION LIMIT
*
WRITE(5,*) 'the lower 95% prediction limit = ', MID, ' liters'
END
```