STATISTICAL DETERMINATION OF PRESERVATIVE THRESHOLD RETENTION IN SOIL BLOCK TESTS

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ABSTRACT

This statistical approach allows estimation of the threshold retention value for preservatives assayed in soil block tests. The threshold value corresponds to 1% (or any other positive value) weight loss from decay only. An associated confidence interval can be given for this threshold estimate, allowing comparison of different preservatives. An "operational" weight loss line is used to adjust the percent weight loss data for loss caused by preservative or solvent evaporation. The adjusted data are then fitted by an exponential or logistic model. Statistical tests for lack of fit are used to test model assumptions. Plots are used to visually judge fitted curves and the estimated threshold preservative retention.

Keywords: Least squares, weighted nonlinear least squares.

INTRODUCTION

Soil block tests are used to gain preliminary indications of the effectiveness of wood preservatives against specified decay fungi. ASTM D 1413-76, "Standard Method of Testing Wood Preservatives by Laboratory Soil Block Cultures," describes the appropriate procedures. In general, g groups (or charges) are used with r replications in each group. The preservative retention in each group is targeted at some level. The results can be displayed graphically as a plot of percent weight loss versus preservative retention (Fig. 1, based on Fig. 3 from ASTM D 1413-76, data from Nance and Amburgey (1976)). In general, percent weight loss decreases as the preservative retention increases. With volatile carriers and high preservative retentions, percent weight loss can start increasing again as the pre-

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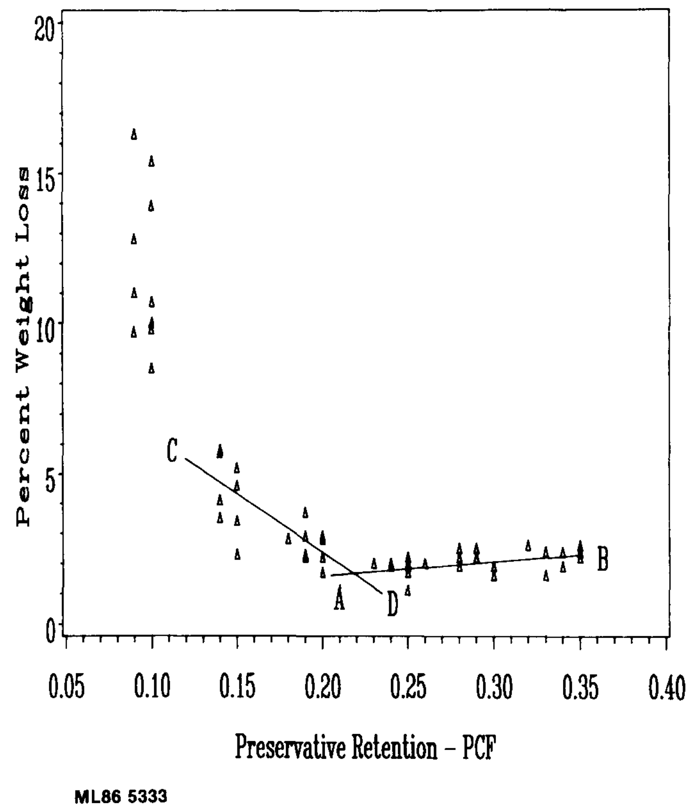

FIG. 1. ASTM D 1413-76. Percent weight loss versus preservative retention (pcf) data with threshold retention defined to be intersection of lines AB and CD. (ML86 5333)

servative retention increases. This is the "operational" weight loss—that caused by the evaporation of the preservative (or solvent) during the course of the experiment. The ASTM standard method for soil block tests employs a visual estimate of the minimum preservative retention (threshold retention) that prevents significant decay. We are proposing a statistical approach that could be used to estimate threshold retentions along with an associated confidence interval.

ASTM PROCEDURE

ASTM D 1413-76 prescribes a visual method of estimating the threshold retention (the minimum amount of preservative retention that prevents significant weight loss caused by decay) by visually fitting a straight line (AB) to the groups that have operational weight loss only, and a straight line (CD) to the other groups that show both weight loss caused by decay and evaporation (Fig. 1). Note that the line CD was not fitted to all the data. The threshold value is then the intersection of these two lines.

A PRIOR STATISTICAL PROCEDURE

Nance and Amburgey (1976) developed one statistical approach to the determination of the operational weight loss. They also gave confidence intervals for a "threshold," which they redefine as a 99% protection level. Their procedure is summarized in the following notation and six steps:

Let the g groups be numbered from 1 to g, from smallest to largest target preservative retention. Note that in Fig. 1 there are g = 6 groups. Also let X = preservative retention, Y = percent weight loss, and Y* = adjusted percent weight loss.

(1) Determine the operational weight loss line. First one must determine which groups are to be included in the operational weight loss line. This procedure assumes that group g will be one of the groups used to fit the operational weight loss line.

(i) Let $k = 1$.

(ii) Using least squares regression, fit the operational weight loss line to data from groups $g - k + 1$ to g.

$$Y = b_1X \tag{1}$$

This is a line with slope b_1, forced through the origin. Call the mean square error s_1^2.

(iii) Using least squares regression, fit a line through the origin to group $g - k$ ($Y = b_2X$). Call the mean square error s_2^2.

(iv) Using Bartlett's test, test the equality of s_1^2 and s_2^2.

(v) If test of equality of variances is not rejected, increase k by 1 and go to (ii). If test of equality of variances is rejected, go to (vi).

(vi) The operational line is fit to groups $g - k + 1$ to g. Using least squares regression, fit a line through the origin to this data ($Y = bX$).

(2) Calculate the adjusted percent weight loss for data in group 1 to $g - k$:

$$Y^* = Y - bX \tag{2}$$

The slope b is the value from step 1 (vi) above. In the ASTM data set, adjusted weight loss values are calculated for groups 1 to 3.

(3) Assume that adjusted percent weight loss decreases exponentially with increased preservative retention. Take logarithms of the adjusted percent weight loss data (throwing out values of adjusted percent weight loss less than 1%).

(4) Using least squares regression, fit a straight line to the logarithms of the adjusted percent weight loss, preservative retention data.

$$\ln(Y^*) = a_0 + a_1X \tag{3}$$

Note: Nance and Amburgey (1976) use base 10 logarithms. The results are comparable (only differing by a constant). We prefer to use natural logarithms because the assumed model is exponential.

(5) Assume that the threshold preservative retention is defined to be the value at 1% adjusted percent weight loss. (The use of 0% adjusted weight loss is impractical, as this is achieved at an infinite preservative retention. Any other positive number could be substituted for 1.) The point estimate of the threshold preservative retention is then equal to $-a_0/a_1$.

(6) Obtain "confidence intervals" on the threshold preservative retention. Least squares regression, as usually used, gives confidence intervals on the dependent variable (here $\ln(Y^*)$) given a value of the independent variable (here X). However, these confidence intervals can be inverted to give "confidence intervals" on the

independent variable given the dependent variable. This is done by taking the points on the usual confidence bands that intersect the horizontal line at the desired value of the dependent variable. These are the values that Nance and Amburgey give in their paper. (Another reference is Draper and Smith 1981, pp. 47–51.) Note that these confidence intervals are confidence intervals on the line, not on individual observations.

We have several concerns about the procedure proposed by Nance and Amburgey. Our primary concern is that emphasis is placed on tests of equality of variance rather than on tests of lack of fit to the hypothesized models. In step 1, groups of data used to determine the operational line should be those groups through which one can fit a straight line through the origin (with a positive slope) with no significant lack of fit, not those groups with equal variances. Tests of equality of variances are sensitive to data that are not normally distributed. Unequal variances in regression problems can be dealt with by weighting. It is inappropriate to compare the mean square error from a regression of a line forced through the origin to data from one group (the $g - k$ group step 1 (iii)) and the mean square error of a regression line forced through the origin to one or more groups (groups $g - k + 1$ to g step 1 (ii)). Equality of mean square errors does not necessarily mean that the same line through the origin will fit both sets of data (groups $g - k$ to g). The mean square error s_1^2 may be "large" if a straight line through the origin does not fit the data in group $g - k + 1$ to g.

In step 3, it is assumed that an exponential model will fit all data sets, although even the authors suggest that a probit or logit model may be more appropriate "where decay loss approaches an upper bound." These models cannot be fit simply by taking logarithms of adjusted percent weight loss and fitting a straight line to the data. Least squares regression also assumes equal error variances, which may not be the case.

When equation (3) is fit to the adjusted data, all adjusted percent weight loss values less than 1% are dropped from the data. These values are dropped because 1) if they are less than zero, they have no logarithms, and 2) if they are close to zero, they can yield large negative values, greatly influencing the resulting regression equation. Therefore, one must extrapolate the fitted line to the 1% level. There are no values less than 1% weight loss to judge the appropriateness of this extrapolation.

The Nance and Amburgey (1976) procedure has worked reasonably well because in general the variability of data from groups that exhibit only operational weight loss is quite small when compared to the variability of groups exhibiting substantial weight loss. The test for equality of variances will be rejected when a group of data with large variability is added to groups of smaller variability, as the resulting error about the regression line will be larger. Also, the increased variability usually occurs with a substantial increase in the percent weight loss, so the slope of the regression line through the origin is substantially changed when this group of data is added for the operational weight loss line calculations, resulting in an increased error about the regression line. In practice, we have come across data sets in which a group of data has low variability, but the percent weight loss in this group is not totally operational. When these data are included in the operational line, (iii), the slope of the regression line changes substantially. However, the test of equality of variances, (iv), is not rejected at the 0.05 level.

OUR PROPOSED STATISTICAL APPROACH

We propose a procedure that allows one to fit an exponential or logistic model to the adjusted percent weight loss, average preservative retention data. Other models could be used, but we have found that if the data do not fit either of these two models, then they are unlikely to fit any other reasonable model. Both these models are asymptotic at zero for large preservative retentions. The logistic model is useful if, at very low preservative retentions, percent weight loss remains constant for a period before decreasing with increased preservative retention. A group of data is left near 0% weight loss, so that the fit at the 1% weight loss might be judged (at least visually).

The primary feature of this approach is the ability to statistically test for lack of fit to hypothesized models at each step. Plots are used at each step to also visually judge the fitted models. Weighting is used so that the statistical tests are appropriate since variability of percent weight loss (or adjusted percent weight loss) in each group is not constant. To test for lack of fit and to determine appropriate weights, one must have replicate values for a given preservative retention. Soil block experiments have no "true" replicates (as the preservative retention is slightly different for each block). However, the preservative retentions in any one group are similar enough that for practical purposes one can use them as true replicates. This is done by using as the independent variable the average preservative retention in the group in place of the individual preservative retention.

One assumption that cannot be tested is the assumption that the operational weight loss fits a straight line through the origin. One could use another model. (The final results are unlikely to vary much as the adjustment usually amounts to less than 1%.) It is reasonable to force the model through the origin. A negative intercept would imply that when one adjusted the percent weight loss data, some values might actually increase.

Given the assumption about the operational weight loss line, the procedure (which is similar to the Nance and Amburgey (1976) procedure) can be outlined in the following five steps:

Again let the g groups be numbered from 1 to g—smallest to largest target preservative retention. Also let X = preservative retention, X^* = average preservative retention in a group, Y = percent weight loss, and Y^* = adjusted percent weight loss. As the procedure is discussed, it will be illustrated with the data of Fig. 1, which is the data set featured in ASTM D 1413-76 and in Nance and Amburgey (1976).

(1) Determine the operational weight loss line. First one must determine which groups are to be included in the operational weight loss line. There are $g = 6$ groups.

(i) Calculate the average and variance of percent weight loss and preservative retention for each group (Table 1).

(ii) Determine $g - k$, such that the average percent weight loss is lowest for group $g - k$. If $k = 0$, no groups are used to fit the operational weight loss line; go to step 2.

Group 4 has the lowest average percent weight loss. Because $g = 6$, $k = 2$.

(iii) Let $j = 1$.

TABLE 1. *Summary statistics for percent weight loss and preservative retention.*

Group	Percent weight loss n_i	Percent weight loss Average	Percent weight loss Variance = V_w	Weight $W = 1/V_w$	Preservative retention Average = X^*	Preservative retention Variance
1	10	11.81	7.001	0.1428	0.096	0.00002667
2	10	4.45	1.407	0.7106	0.144	0.00002667
3	10	2.57	0.316	3.1679	0.194	0.00004889
4	10	1.85	0.092	10.9091	0.247	0.00006778
5	10	2.17	0.089	11.2360	0.289	0.00005444
6	9	2.28	0.109	9.1371	0.340	0.00012500

(iv) Using weighted least squares, fit a line through the origin to the percent weight loss, average preservative retention data from groups $g - k$ to $g - k + j$. The weight for an observation (Table 1) is inversely proportional to the variance of percent weight loss for that group, i.e., $W = 1/V_w$. (See appendix for details about fitting a weighted least squares model.)

The weighted least squares line fitted through the origin to data from groups 4 and 5 has a slope of 7.5009.

(v) Using the residuals from the model fitted in (iv), test for lack of fit. (See appendix for details about testing for lack of fit.)

The F statistic to test lack of fit is 0.0014 on 1 and 18 degrees of freedom, which gives a p value of 0.9709 which is not significant at any reasonable level.

(vi) If the hypothesis of no lack of fit is accepted and $j < k$, increase j by 1 and go to (iv). If the hypothesis of no lack of fit is accepted and $j = k$, increase j by 1 and go to (vii). If the hypothesis of no lack of fit is rejected, go to (vii).

The hypothesis of no lack of fit is accepted, and as j (equal to 1) is less than k (equal to 2), j is increased by 1, and we go back to (iv).

Repeat (iv). The variable j is now equal to 2. The weighted least squares line fitted through the origin to data from groups 4 to 6 is 7.2026. Repeat (v). The F statistic to test lack of fit is 1.9179 on 2 and 26 degrees of freedom, which gives a p value of 0.1671 and is not significant at the 0.05 level. Repeat (vi). The hypothesis of no lack of fit is accepted, and as $j = k = 2$ we increase j to 3 and go to (vii).

(vii) Using weighted least squares, fit the operational weight loss line to the percent weight loss, average preservative retention data from groups $g - k$ to $g - k + j - 1$. (This is one of the lines previously fitted in (iv).) Call the slope of this fitted model b. If $b < 0$, no adjustment is taken; set b equal to 0 and go to step 2. If $j = 1$, the operational weight loss line is fitted through the origin and the group of data with the lowest average percent weight loss. If this average is negative, which has occurred in actual data sets, then the slope will also be negative. Because this is contrary to theory, no adjustment is taken. Plot the fitted operational weight loss line with the percent weight loss and average preservative retention data from all groups to visually look at the fit.

The operational weight loss line is fitted to groups 4 to 6 using weighted least squares. The slope, b, is 7.2026. The plot of the data with the fitted operational weight loss line (Fig. 2) gives no reason to reject the fitted line.

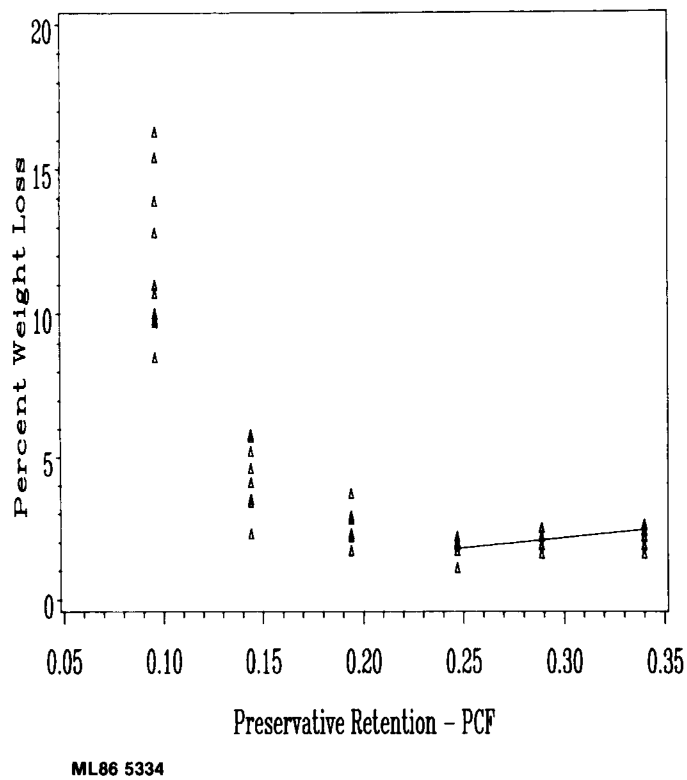

FIG. 2. ASTM D 1413-76. Percent weight loss versus average preservative retention (pcf) data with fitted operational weight loss line. (ML86 5334)

(2) Calculate the adjusted percent weight loss for data in group 1 to g − k using the average preservative retention:

$$Y^* = Y - bX^* \tag{4}$$

Note that this differs from the Nance and Amburgey (1976) procedure in that here one keeps the first group of data used to fit the operational weight loss line in the adjusted data set. This group has adjusted percent weight loss values near zero and is used to judge the fit of the subsequent exponential or logistic model. Also, we have used the average preservative retention in a group in place of the individual preservative retention. Some of the adjusted percent weight loss data may have negative values. This is no cause for concern, and these data should not be eliminated from the analysis.

In this example, the adjusted percent weight loss is calculated for groups 1 to 4 by $Y^* = Y - 7.2026X^*$.

(3) Using weighted nonlinear least squares, fit an exponential and logistic model to the adjusted percent weight loss and average preservative retention data. See appendix for details about fitting a weighted nonlinear least squares model. The weights are the inverses of the variances of the adjusted percent weight loss data for each group. These are the same values W as in step 1 (iv). (The variance of the percent weight loss data equals the variance of the adjusted percent weight

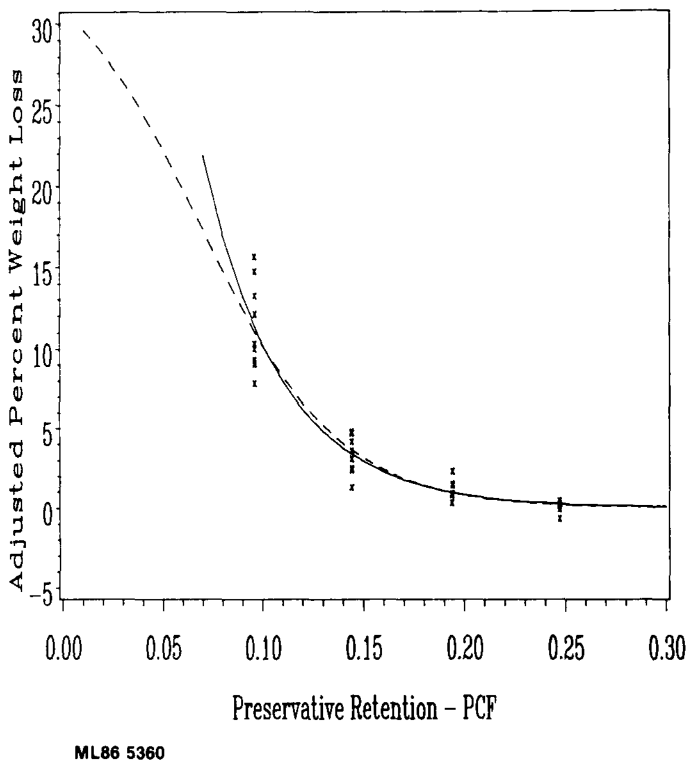

FIG. 3. ASTM D 1413-76. Adjusted percent weight loss versus average preservative retention (pcf) data with fitted exponential (solid line) and logistic (dashed line) models. (ML86 5360)

loss data, as the adjustment is a constant value within any given group.) The equation for an exponential model is

$$Y^* = \exp(c_0 - c_1X^*) \tag{5}$$

and for a logistic model

$$Y^* = d_0(1 - (1/(1 + \exp(d_1 - d_2X^*)))) \tag{6}$$

Note: At least two groups of data are needed to fit the exponential model (as there are two parameters to estimate), and at least three groups are needed to fit the logistic model. The logistic model may be difficult to fit if there appears to be no upper bound on the adjusted percent weight loss data. In this case, one may wish to consider only the exponential model. Plot the exponential and logistic fits along with the adjusted percent weight loss, average preservative data from groups 1 to $g - k$ to visually judge the fit.

Although there is little sign of an upper bound on adjusted percent weight loss, we were able to fit a logistic model to the data. The fitted equations were

exponential: $Y^* = \exp(4.8858 - 25.3054X^*)$
logistic: $Y^* = 34.907(1 - (1/(1 + \exp(1.9966 - 28.854X^*))))$

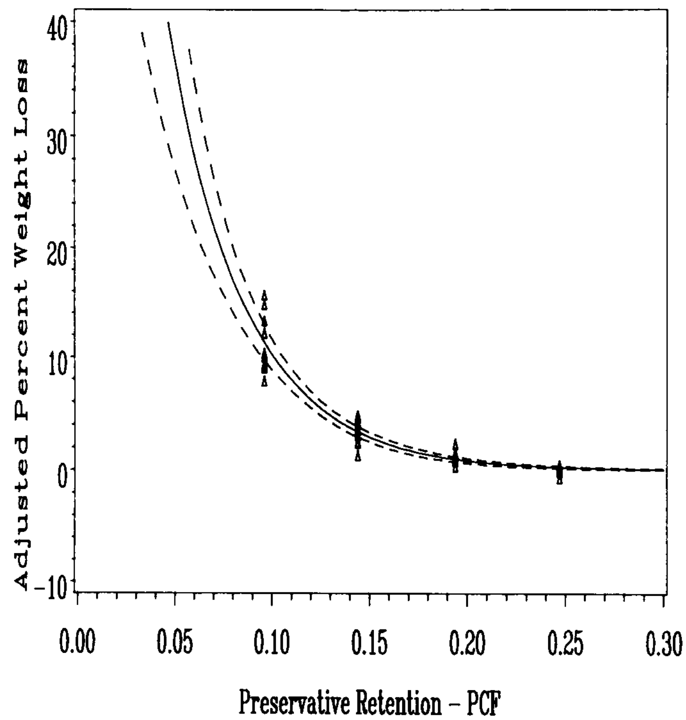

FIG. 4. ASTM D 1413-76. Adjusted percent weight loss versus average preservative retention (pcf) data with fitted exponential model (solid line) and confidence intervals (dashed lines). (ML86 5335)

The fitted models are plotted with the data in Fig. 3. (The exponential model is the solid line, and the logistic model is the dashed line.)

(4) Using the residuals from the fitted model, test for lack of fit to the exponential or logistic model (see appendix for details). Note: At least three groups of data are needed to test for lack of fit to the exponential model, and at least four groups are needed for the logistic model. Even if statistically there is lack of fit, visually judge if that lack of fit is at high or low adjusted percent weight loss values. There should be a group of data near 0% weight loss. Does the fitted model appear to fit well in this area?

For the exponential model, the F statistic to test for lack of fit is 2.5449 with 2 and 36 degrees of freedom, which gives a p value of 0.0925. For the logistic model, the F statistic to test for lack of fit is 4.1709 with 1 and 36 degrees of freedom, which gives a p value of 0.0485. Looking at Fig. 3, it appears that either model fits the low percent weight loss values adequately.

(5) Calculate the upper and lower confidence bounds for the fitted model (see appendix). Plot the fitted line and upper and lower confidence bands from a given model with the data from groups 1 to g − k. The intersection of the line $Y^* = 1$ with the fitted model gives a point estimate of the threshold preservative retention at the 1% weight loss value (any other positive value could be chosen). The intersection of the line $Y^* = 1$ with the upper and lower confidence bounds for

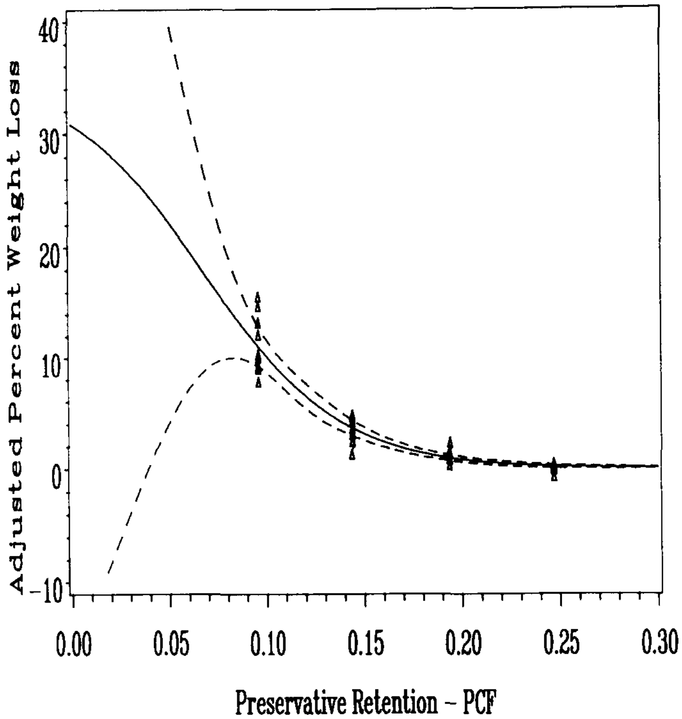

FIG. 5. ASTM D 1413-76. Adjusted percent weight loss versus average preservative retention (pcf) data with fitted logistic model (solid line) and confidence intervals (dashed line). (ML86 5336)

the fitted model gives a confidence interval for the threshold preservative retention value. Again these are confidence bounds on the fitted model, not an individual observation.

The fitted model (solid line) with the associated upper and lower confidence bounds (dashed lines) are plotted in Fig. 4 (exponential) and Fig. 5 (logistic). The intersection of these curves with the line $Y^* = 1$ gives the point estimate and associated confidence interval for the threshold preservative retention.

Model	Point estimate (confidence interval)
Exponential	0.1919 (0.1819 – 0.2016)
Logistic	0.1914 (0.1821 – 0.2015)

In this case, the two models give similar estimates, which is to be expected as the fit is similar for small values of percent weight loss.

ADDITIONAL EXAMPLE

The second example is a sequence of weight loss data from a soil block test in which southern pine sapwood blocks were treated to a series of retentions of water-soluble pentachlorophenol in a methanol, AMINE PMT® solution and were decayed by *Coniophora puteana* (Schum. ex Fr.) Karst. A plot of the data is given

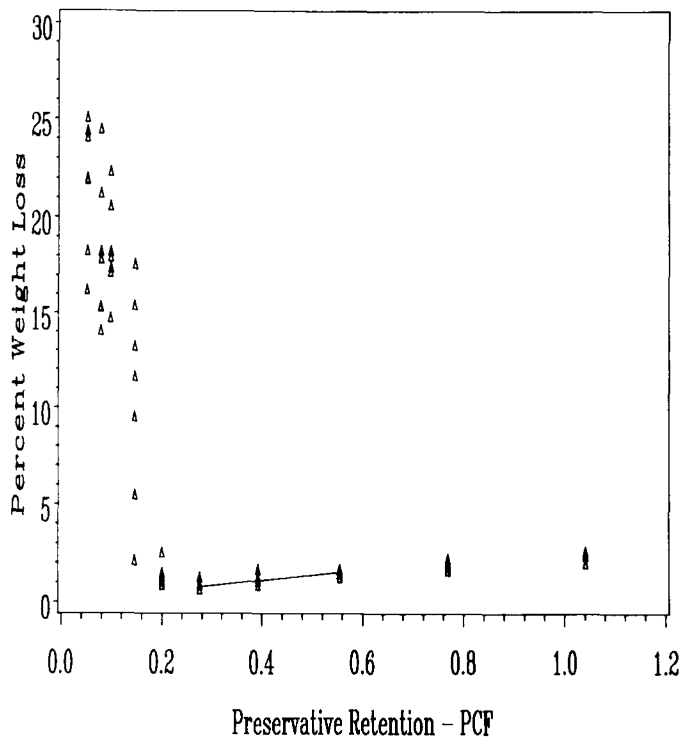

FIG. 6. Example 2. Percent weight loss versus average preservative retention (pcf) data with fitted operational weight loss line. (ML86 5337)

in Fig. 6. The percent weight loss does not decrease very quickly for the first three groups, which means that the exponential model is not likely to fit well. There are 10 groups of data. The lowest average percent weight loss is in group 6. The lack of fit tests for the operational weight loss line in step 1 (v) can be summarized as follows:

Groups	p value
6 to 7	0.8831
6 to 8	0.0598
6 to 9	0.0424
6 to 10	0.0011

Using the 5% level of significance, one would use groups 6 to 8 to fit the operational weight loss line. (One could make arguments for using groups 6 to 7 or groups 6 to 9, but one would not want to include group 10.) This fitted operational weight loss line is also shown in Fig. 6. Again, there appears to be no reason to reject this fitted line.

Exponential (solid line) and logistic (dashed line) models were fit to these data (Fig. 7). The exponential model does not appear to fit the data at all, while the logistic appears to give a reasonable fit. This is borne out by the statistical tests of lack of fit. The p value for testing lack of fit to the exponential model is less

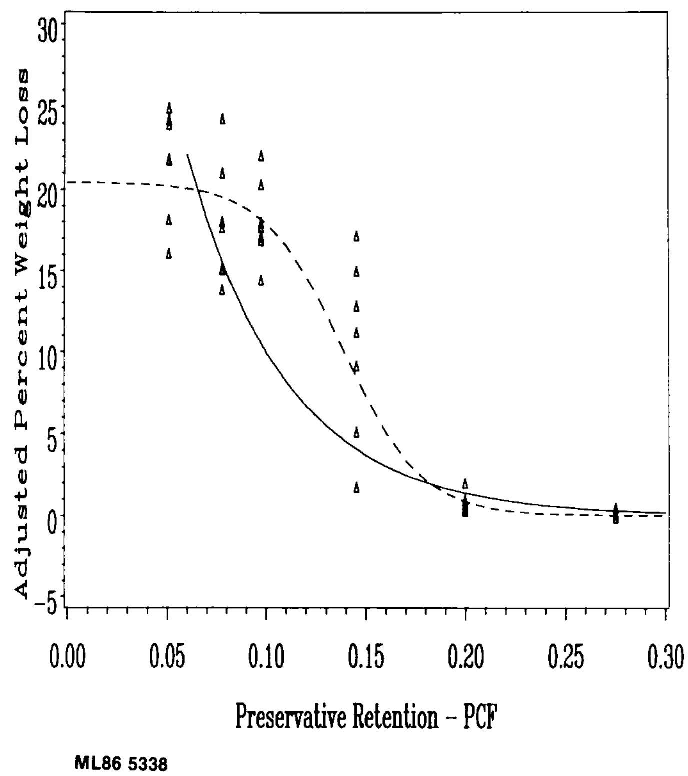

FIG. 7. Example 2. Adjusted percent weight loss versus average preservative retention (pcf) data with fitted exponential (solid line) and logistic (dashed line) models. (ML86 5338)

than 0.0001, and the p value for testing lack of fit to the logistic model is 0.1602. Therefore, one would only calculate confidence bands about the logistic fit (Fig. 8). The point estimate for the threshold preservative retention is 0.1963, and a 95% confidence interval for this value would be 0.1850 to 0.2053.

CONCLUSIONS

We propose a statistical method that includes provisions to test for lack of fit to assumed models for determining preservative threshold retention in soil block experiments. Although the threshold has been defined in this paper to indicate the preservative retention that results in 1% weight loss caused by decay, any other nonzero value could be chosen. In addition, plots are used to visually assess the goodness of fit of the models. By including a group of data near 0% weight loss, one can visually judge the resulting point estimate and associated confidence interval for the threshold preservative retention.

The use of weighting eliminates the need for transformations of the data to ensure homogeneity of variances. A logistic model (in addition to the exponential model) is proposed for situations in which there appears to be an upper bound on the percent weight loss for small levels of preservative retention. Confidence bands are given on the fitted exponential or logistic model, which one can invert to give confidence bounds on the threshold preservative retention.

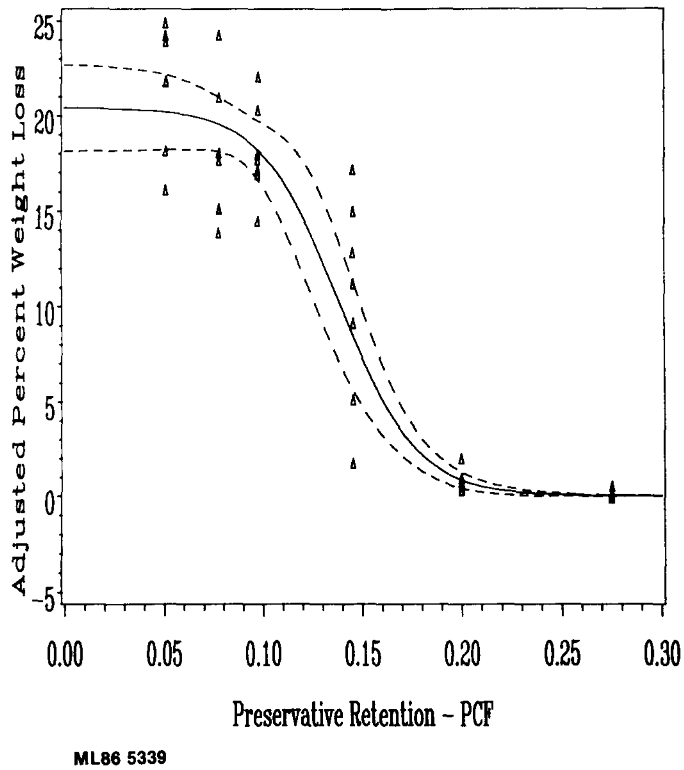

FIG. 8. Example 2. Adjusted percent weight loss versus average preservative retention (pcf) data with fitted logistic model (solid line) and confidence intervals (dashed line). (ML85 5339)

We think that this statistical approach to estimating threshold values, along with the appropriate confidence intervals, will enable better comparisons of candidate compounds than the ASTM D 1413-76 visual method.

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APPENDIX—STATISTICAL DETAILS

Notation

For a given analysis, let there be m groups of data of n_i observations in each group, i equals 1 to m. The groups are ordered 1 to m with increasing value of the average preservative retention. There are a total of N observations ($N = n_1 + \ldots + n_m$). For example from our proposed statistical approach, there are $j + 1$ groups of data when fitting the operational line through the origin, step 1 (iv), and $g - k$ groups when fitting the exponential or logistic models in step 3. Let x be the independent variable (average preservative retention for this study) and y the dependent variable (either percent weight loss when estimating the operational weight loss line or adjusted percent weight loss when fitting the exponential or logistic model).

TABLE A1. *Model equations and parameters for weighted least squares.*

Model	Equation = f(x)	p_0	p_1	p_2	Number of parameters (p + 1)
Operational	$y = bx$	b			1
Exponential	$y = \exp(c_0 - c_1x)$	c_0	c_1		2
Logistic	$y = d_0(1 - (1/(1 + \exp(d_1 - d_2x))))$	d_0	d_1	d_2	3

Weighted least squares

Let f(x) represent the model to be fitted and $p_o, \ldots, p_p$ represent the parameters to be fitted, i.e., one is fitting p + 1 parameters (Table A1). Weighted least squares finds parameter estimates such that the weighted residual sum of squares error (SSE) is minimized:

$$SSE = \Sigma\, W(y - f(x))^2$$

Many computer packages will do weighted least squares regression. For example, see the GLM (general linear model) procedure in SAS[2] for linear regressions and the NLIN (nonlinear regression) procedure.

Test of lack of fit

Use the weighted sum of squares for the model (A) and error (B) that are given in the regression package and complete Table A2. The F statistic to test lack of fit to a given model is $(B - N + m)/(m - p - 1)$ with $m - p - 1$ and $N - m$ degrees of freedom.

Confidence bands for the exponential and logistic models

The output from the nonlinear regression program should include estimates of the standard errors and correlations of the parameter estimates. Use these estimates to form a (p + 1) by (p + 1) covariance matrix, S. Approximate upper and lower $100(1 - \alpha)$ percent confidence bounds on f(x) are then given by:

$$f(x) \pm z_{(\alpha)}\sqrt{(D'SD)}$$

where $z_{(\alpha)}$ is a value from a standard normal distribution (mean 0, variance 1) such that the probability that a standard normal random variable lies between $\pm z$ with probability $1 - \alpha$; and D is a p + 1 by 1 matrix of partial derivatives of f(x) with respect to each parameter.

For the specific cases under consideration here, D'SD can be written as:

exponential:

SEA = standard error of c_0
SEB = standard error of c_1
RAB = correlation of c_0 and c_1
DA = partial derivative with respect to $c_0 = \exp(c_0 - c_1x)$
DB = partial derivative with respect to $c_1 = -x\exp(c_0 - c_1x)$

$$D'SD = (DA\ SEA)^2 + (DB\ SEB)^2 + 2(DA\ SEA\ RAB\ DB\ SEB)$$

logistic:

SEA = standard error of d_0
SEB = standard error of d_1
SEC = standard error of d_2
RAB = correlation of d_0 and d_1
RAC = correlation of d_0 and d_2
RBC = correlation of d_1 and d_2

[2] SAS Institute. 1985. Statistical analysis system (SAS) user's guide: Statistics. SAS Institute, Cary, NC.

TABLE A2. *Analysis of variance for testing lack of fit.*

Source	Sum of squares	df[1]	Mean square	*F* statistic
Model	A	p + 1		
Error	B	N − p − 1		
Pure error	N − m	N − m	1.0	
Lack of fit	B − N + m	m − p − 1	(B − N + m)/(m − p − 1)	(B − N + m)/(m − p − 1)

[1] df = degrees of freedom.

$TT = 1 + \exp(d_1 - d_1 x)$

DA = partial derivative with respect to $d_0 = (1 - (1/(1 + \exp(d_1 - d_2 x))))$

DB = partial derivative with respect to $d_1 = d_o \exp(d_1 - d_2 x)/TT^2$

DC = partial derivative with respect to $d_2 = -d_0 \times \exp(d_1 - d_2 x)/TT^2$

$$D'SD = (DA\ SEA)^2 + (DB\ SEB)^2 + (DC\ SEC)^2 + 2(DA\ SEA\ RAB\ DB\ SEB) + 2(DA\ SEA\ RAC\ DC\ SEC) + 2(DB\ SEB\ RBC\ DC\ SEC)$$