Published online August 25, 2005

Brittle Fracture of Soil Aggregates: Weibull Models and Methods of Parameter Estimation

L. Munkholm* and E. Perfect

ABSTRACT

Brittle fracture of soil aggregates is usually analyzed with the Weibull "weakest-link" model. Failure is expressed in terms of a probability distribution function (pdf) of aggregate strengths. Traditionally a two-parameter Weibull model is fitted to double log-transformed data with the Weibull parameters (α and β) estimated using linear regression. The main objective of this study was to compare the goodness-of-fit for a three-parameter versus a two-parameter Weibull model. In addition, we compared three common methods of parameter estimation: linear regression, nonlinear regression, and maximum likelihood. The different models and methods of estimation were evaluated using previously published and unpublished aggregate rupture energy data from three contrasting soil types (Bygholm sandy loam, Maury silt loam, and Karnak silty clay). Overall, the goodness-of-fit was not markedly improved by using a three-parameter as compared with a two-parameter Weibull model. The choice of model had a significant effect on the parameter estimates. The three-parameter model produced lower estimates of β than the two-parameter model. The data were always best fitted using nonlinear regression. Nonlinear regression also resulted in a greater power of distinction between management treatments and aggregate sizes for α on the Maury soil. We recommend fitting aggregate rupture data to a two-parameter Weibull model and estimating the model parameters using nonlinear regression.

Brittle fracture of soil aggregates is often analyzed probabilistically to investigate soil, management, and/or size effects. Several different probabilistic models have been proposed for the brittle fracture of heterogeneous materials (e.g., Srolovitz and Beale, 1988; Herrmann and Roux, 1990; Frantziskonis, 1995). Of these, the Weibull "weakest-link" model (Weibull, 1952; Freudenthal, 1968) is the most widely accepted. Failure in this model is expressed in terms of a pdf of aggregate strengths.

The Weibull distribution may be expressed as a two-parameter model, with scale (α) and shape (β) parameters, or as a three-parameter model that also includes a location parameter (E_0). The two-parameter Weibull model implies that the probability of failure is zero only when the rupture energy (E) is zero, that is, there is always a probability to fail no matter how small the rupture energy. Shih (1980) suggested using a three-parameter model to characterize the pdf of strengths for brittle materials to obtain a better goodness-of-fit to experimental data. To our knowledge the three-parameter model has not been previously applied to characterize brittle fracture of soil aggregates.

Double logarithmic transformation of an aggregate strength pdf combined with linear regression (LIN) is the standard parameter estimation method in soil studies (Braunack et al., 1979; Dexter and Watts, 2000). Lack of a straight line fit is a common problem in soil studies (Perfect et al., 1998). This indicates problems with model and/or fitting method. For other applications, the LIN method has been questioned and the maximum likelihood method (ML) has been shown to provide more accurate parameter estimates for the two-parameter model (Trustrum and Jayatilaka, 1979; Khalili and Kromp, 1991; Seguro and Lambert, 2000; Clarke, 2003). In a few studies, Weibull parameters have been estimated using nonlinear regression (NLIN) (Perfect and Kay, 1994; Perfect et al., 1998). The NLIN method has also been applied to the three-parameter model (Ferreira et al., 2003). A number of other methods of parameter estimation have been proposed. The method of moments is probably the most well known of the alternative approaches. However, previous studies have shown that this method does not provide more accurate estimates than the more common LIN and ML methods (Trustrum and Jayatilaka, 1979; Mahdi and Ashkar, 2004).

The main objective of this study was to evaluate the applicability of a three-parameter versus a two-parameter Weibull model to fit to soil-aggregate brittle fracture data. An additional objective was to compare three common methods of parameter estimation: LIN, NLIN, and ML. The different models and methods of estimation were evaluated using measured aggregate rupture energy data from three contrasting soil types: Bygholm sandy loam, Maury silt loam, and Karnak silty clay. The Bygholm and Maury data sets have been reported in previous papers (Perfect et al., 1998; Munkholm and Kay, 2002; Munkholm and Schjønning, 2004). The Karnak data have not been previously published. We evaluated the goodness-of-fit, effects on parameter estimates, and power of discrimination between management treat-

L. Munkholm, Dep. of Agroecology, Danish Institute of Agricultural Sciences, Research Centre Foulum, P.O. Box 50, DK-8830 Tjele, Denmark; E. Perfect, Dep. of Earth and Planetary Sciences, Univ. of Tennessee, 1412 Circle Dr., Knoxville, TN 37996. Received 30 Aug. 2004. *Corresponding author (lars.munkholm@agrsci.dk).

Published in Soil Sci. Soc. Am. J. 69:1565–1571 (2005).
Soil Physics
doi:10.2136/sssaj2004.0290

Abbreviations: AIC, Akaike's information criterion; ANOVA, analysis of variance; cdf, cumulative probability density function; D, Kolmogorov-Smirnov statistic; E, rupture energy; E_0, the location parameter—the value of E where the probability of failure is estimated to be zero; F, Fisher's F statistic; L, likelihood function; LIN, linear regression; LIN-2 = linear regression, two-parameter Weibull model; ML, maximum likelihood; ML-2, maximum likelihood, two-parameter Weibull model; ML-3, maximum likelihood, three-parameter Weibull model; n, number of fits or samples; NLIN, nonlinear regression; NLIN-2, nonlinear regression, two-parameter Weibull model; NLIN-3, nonlinear regression, three-parameter Weibull model; P, probability; pdf, probability density function; R^2, coefficient of determination; RSS, residual sums of squares.

ments for the different models and methods of parameter estimation.

THEORY

Weibull Models

According to the most widely used Weibull model, the probability of survival for a population of identically sized soil aggregates is given by (Perfect and Kay, 1995):

$$P(E \leq E_i) = 1 - \exp[-(E_i/\alpha)^{\beta}] \quad [1]$$

where $P(E \leq E_i)$ is the cumulative probability density function (cdf), E is rupture energy, E_i is specified rupture energy, α is the characteristic strength of the population, corresponding to the 63rd percentile of the cdf for E, and β characterizes the spread of rupture energies around α. Utomo and Dexter (1981) used the reciprocal of β as an index for soil friability and proposed threshold values for poor to good friability.

An offset point larger than zero can be included in the standard Weibull distribution, making it a three-parameter model (Shih, 1980):

$$P(E \leq E_i) = 1 - \exp\{-[(E_i - E_0)/(\alpha - E_0)]^{\beta}\} \quad [2]$$

where E_0 is a location parameter, that is, the value of E where the probability of failure is estimated to be zero.

The probability of survival in Eq. [1] and [2] is usually approximated by (Braunack et al., 1979):

$$P(E \leq E_i) = m/(n + 1) \quad [3]$$

where m is the rank (in ascending order) of each measurement of E within a size fraction and n is the total number of samples for that fraction. Other methods of calculating $P(E \leq E_i)$ have also been proposed (e.g., Khalili and Kromp, 1991; Perfect et al., 1998). However, it was not our goal to evaluate these different approaches.

Estimation of Model Parameters

Based on the cdf data, the Weibull parameters may be estimated using LIN and NLIN. The two-parameter Weibull distribution, Eq. [1], can be written in linear form by taking the logarithm twice:

$$\ln\{-\ln[1 - P(E \leq E_i)]\} = \beta\ln(\alpha) - \beta\ln(E_i) \quad [4]$$

The parameters can then be estimated by applying the LIN method, that is, linear regression using the least squares procedure, with β equal to the slope and α equal to 2.718… raised to the power of the intercept divided by β. This method is also known as the "graphical method" or the "method of least squares." The LIN method is restricted to parameter estimation for the two-parameter model, since the three-parameter model cannot be linearized.

The Weibull parameters in Eq. [1] may alternatively be estimated by nonlinear regression, NLIN (SAS Institute, 1999). This method produces least square estimates of the parameters of a nonlinear model. The NLIN method can also be used to estimate parameters for the three-parameter Weibull model.

For the ML method, the Weibull parameters are estimated based on the pdf rather than the cdf. In ML, the Weibull parameters are derived as the values that maximize the likelihood function, L (e.g., Khalili and Kromp, 1991):

$$L = \prod_{i=1}^{n} f(E_i) \quad [5]$$

where $f(E_i) = dP(E \leq E_i)/dE_i$ and n is the number of samples. Maximizing L is equal to maximizing the log L function.

MATERIALS AND METHODS

Soils and Brittle Fracture Measurements

Aggregate strength data were analyzed for three different soils: Bygholm sandy loam (Oxyaquic Agriudoll), Maury silt loam (Typic Paludalf), and Karnak silty clay (Vertic Endoaquept). The Bygholm samples were taken from two traffic compaction experiments (I and II) located on the organically managed Rugballegård Experimental Station, Denmark (Munkholm and Kay, 2002; Munkholm and Schjønning, 2004). In both experiments a compaction treatment was compared with a reference treatment. From Exp. I samples were taken at the 7- to 12-cm depth. Additional information regarding Exp. I can be found in Munkholm and Kay (2002). For Exp. II the soil was sampled from the 0- to 5-cm depth in a randomized block experiment with three replicates. Soil was sampled after compaction and before secondary tillage in six 0.5-m^2 areas in each plot. Subsequently, the subsamples from each plot were bulked. The bulked samples were air-dried and separated into different aggregate-size classes: 4 to 8 and 8 to 16 mm (Exp. I), and 8 to 16 and 16 to 32 mm (Exp. II) as described in Munkholm and Kay (2002). Fifteen aggregates were then selected from each size fraction and replication (i.e., 45 per treatment and size fraction).

The Maury samples were collected from a long-term tillage experiment at the University of Kentucky Experiment Station research farm, near Lexington, KY, USA. The experimental design and its influence on soil properties have been described previously (Perfect and Blevins [1997] and references therein). Two corn (*Zea mays* L.) management practices with conventional N fertilizer application rates were sampled: till (moldboard plowed to a depth of 20 to 25 cm, plus disked to a depth of 8 to 10 cm each spring) and no-till (no plowing or disking). The conventional-till plots were sampled immediately after plowing and again after two passes with a disk harrow. Each treatment was replicated four times. Details on sampling are given in Perfect et al. (1998). In the laboratory the soil samples were air-dried and separated into three size classes: 4 to 8, 8 to 16, and 16 to 31.5 mm (Perfect et al., 1998). Forty aggregates were chosen at random from each sieved fraction of each replication and tillage treatment.

The Karnak samples were taken from a long-term (>5 yr) no-till field at Elks Creek Farms, Hopkins County, KY, USA. The crop at time of sampling was soybean [*Glycine max* (L) Merr.]. Samples were collected from the 0- to 10-cm depth of non-trafficked interrows at three replicate locations as described by Perfect et al. (1997). The samples were air-dried and separated into three size classes: 4 to 8, 8 to 16, and 16 to 31.5 mm using a nest of sieves, shaken for 60 s at a 2-mm amplitude on a Fritsch (model: Analysette 3) vibratory sieve shaker. Forty aggregates were chosen at random from each sieved fraction of each replication.

The selected aggregates were crushed individually between two flat parallel plates using the indirect tension test (Perfect et al., 1998; Munkholm and Kay, 2002). The E was computed automatically by integrating the force-displacement curve up to the point of failure and dividing the result by the aggregate mass (Perfect and Kay, 1994). Generally a linear stress–strain relationship until failure was found and the aggregates broke into two halves along the vertical axis. This indicates that tensile failure was the dominant mode of failure (i.e., no indication of substantial plastic deformation until failure).

Data Analysis

The $P(E \leq E_i)$ were calculated from the measured rupture energies using Eq. [3]. The ranking was performed for data from individual plots for the Karnak and Maury sites, that is, 40 samples per plot and size. For the Bygholm site, the data for each combination of trial, treatment, and size were pooled to provide an adequate number of samples for parameter estimation (i.e., 45 samples after pooling). The number of samples was markedly higher than the minimum number of samples recommended by Dexter and Watts (2000) ($n > 10$) and Perfect et al. (1998) ($n > 20$) for brittle fracture studies.

Equation [4] was fitted to the $P(E \leq E_i)$ and E data by linear regression (PROC GLM; SAS Institute, 1999), yielding LIN parameter estimates for the two-parameter Weibull distribution (LIN-2). Equations [1] and [2] were fitted to the same data using nonlinear regression analysis (PROC NLIN; SAS Institute, 1999). This gave nonlinear regression estimates for the two- and three-parameter Weibull models (labeled NLIN-2 and NLIN-3, respectively). The GAUSS method was applied for iterative estimation of a nonlinear model in the NLIN method (SAS Institute, 1999). The E_0 parameter was bounded to be between 0 and the minimum observed E value when nonlinear regression was used to fit Eq. [2]. All of the fits converged according to the software default criterion (SAS Institute, 1999). Maximum likelihood estimates were also computed for two- and three-parameter Weibull models (ML-2 and ML-3, respectively) using PROC CAPABILITY (SAS Institute, 1999). This procedure uses a Newton-Raphson algorithm to maximize the log-likelihood function ($\log L$) with respect to the regression parameters.

Goodness-of-fit was evaluated by comparing the observed and predicted cdf curves using the Kolmogorov-Smirnov statistic (SAS Institute, 1999). The Kolmogorov D value was estimated by:

$$D = \max|[P(E \leq E_i)_{obs} - P(E \leq E_i)_{pred})| \qquad [6]$$

where $P(E \leq E_i)_{obs}$ and $P(E \leq E_i)_{pred}$ are the observed and predicted cdf values at E_i. The D values were calculated using PROC INSIGHT (SAS Institute, 1999). Probability (P) values were also computed, where P is the probability of obtaining a D statistic greater than the computed D statistic when the null hypothesis is true (SAS Institute, 1999). The null hypothesis is that the data come from a Weibull distribution with given α, β, and E_0 values. The smaller the P value, the stronger the evidence against the null hypothesis. The D values (i.e., one per dataset per site [e.g., $n = 36$ for Maury]) were subsequently used for statistical analysis of model/estimation method effects using analysis of variance (ANOVA) and comparison of means techniques in PROC GLM (SAS Institute, 1999). For estimates of α, β, and E_0 similar analysis of model/estimation method effects were performed. For the Maury soil, parameter estimates were statistically analyzed for treatment and size effects using ANOVA. This analysis was performed for each method to obtain a measure of the power of discrimination between treatments for the different models/estimation methods. F-values from the ANOVA were used as indicators of the power of discrimination. The balance between goodness-of-fit and parsimony for the different models was evaluated using Akaike's information criterion (AIC) applied to the NLIN and ML methods. The AIC was estimated by (SAS Institute, 1999):

$$\mathrm{AIC} = n\ln(\mathrm{RSS}/n) + 2p \qquad [7]$$

where n is the number of observations, RSS is the residual sums of squares and p is the number of model parameters. The smaller (more negative) the AIC value, the better the model. The AIC values (i.e., one per dataset) were subsequently used for statistical analysis of model/estimation method effects using analysis of variance (ANOVA) and comparison of means techniques in PROC GLM (SAS Institute, 1999).

RESULTS

Goodness-of-Fit

For Bygholm sandy loam, the ML-3, NLIN-2, and NLIN-3 methods gave a significantly ($P < 0.05$) better goodness-of-fit (i.e., lower D values) than the ML-2 and LIN-2 methods (Fig. 1A). The NLIN-3 method resulted in the lowest D value. However, this value was not significantly different from those for the NLIN-2 and ML-3 methods. The P values indicated that the methods ranked in the order (i.e., best to worst): NLIN-3 > NLIN-2 > ML-3 > ML-2 > LIN-2 (Table 1). In 7 out of 8 cases the NLIN-3 method gave P values >90% whereas for LIN-2 and ML-2 this only occurred in 1 out of 8 cases. The mean AIC was lowest (most negative) for the NLIN-3 method and highest for ML-3 (Table 2).

The Maury silt loam produced a similar goodness-of-fit ranking for the different estimation methods (Fig. 1B). The two NLIN methods gave significantly ($P < 0.05$) lower D values than the other methods. The ML-3 method was no better than the LIN-2 and ML-2 methods in this case. The P values from the individual fits resulted in

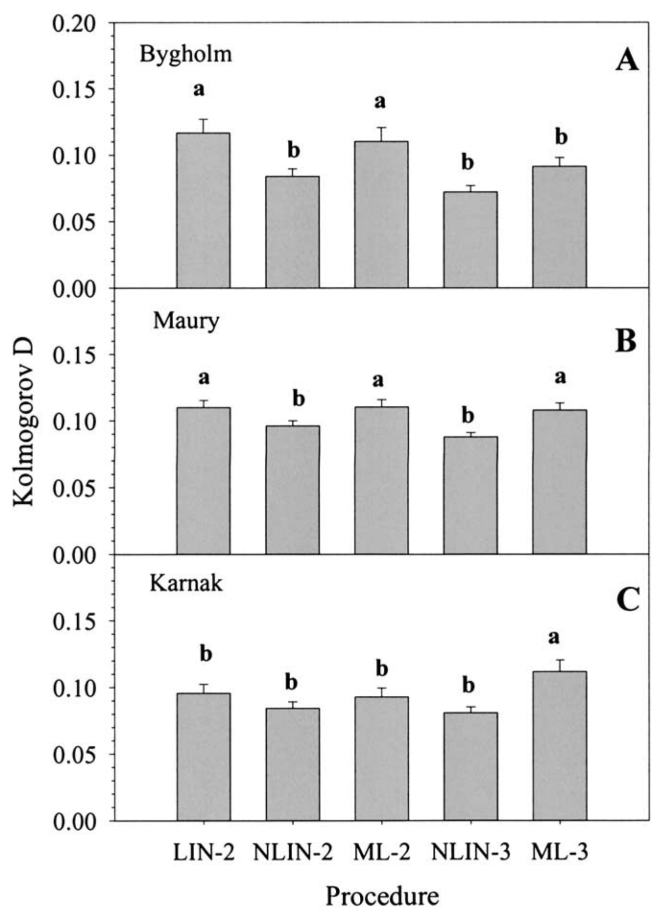

Fig. 1. Kolmogorov D values estimated for the different methods using data for the (A) Bygholm, (B) Maury, and (C) Karnak soils. LIN-2 = linear regression, two-parameter Weibull model; NLIN-2 = nonlinear regression, two-parameter Weibull model; ML-2 = maximum likelihood, two-parameter Weibull model; NLIN-3 = nonlinear regression, three-parameter Weibull model; ML-3 = maximum likelihood, three-parameter Weibull model. Bars indicate standard error of mean. Columns with the same letter within a soil are not significantly different at $P < 0.05$ according to t test.

Table 1. Frequency of tests within *P*-level classes for the different models and estimation methods.

		Number of tests in *P*-level class‡				
Soil	*P*-level†	LIN-2	NLIN-2	ML-2	NLIN-3	ML-3
Bygholm	<70%	6	1	5	0	3
n = 8	70–90%	1	3	2	1	2
	>90%	1	4	1	7	2
Maury	<70%	17	11	17	6	16
n = 36	70–90%	7	12	9	10	10
	>90%	12	13	10	20	9
Karnak	<70%	2	0	2	0	5
n = 9	70–90%	4	2	2	1	2
	>90%	3	7	5	8	2

† *P* is the probability that Kolmogorov *D* is larger than the estimated Kolmogorov *D*.
‡ LIN-2 = linear regression, two-parameter Weibull model; NLIN-2 = nonlinear regression, two-parameter Weibull model; ML-2 = maximum likelihood, two-parameter Weibull model; NLIN-3 = nonlinear regression, three-parameter Weibull model; ML-3 = maximum likelihood, three-parameter Weibull model.

the following ranking: NLIN-3 > NLIN-2 > LIN-2 = ML-2 = ML-3. The methods gave $P > 90\%$ in 56, 36, 33, 28, and 25% of the tests for NLIN-3, NLIN-2, LIN-2, ML-2, and ML-3, respectively (Table 1). In more than 40% of the cases, the LIN-2, ML-2, and ML-3 methods resulted in P values of <70%. The mean AIC estimates decreased in the order ML-3 > ML-2 > NLIN-2 = NLIN-3 (Table 2).

For Karnak silty clay, the NLIN-3 method performed best overall, although the resulting D value was not significantly different ($P < 0.05$) from the D values obtained using the LIN-2, ML-2, and NLIN-2 methods (Fig. 1C). The good performance of the NLIN-3 method was underlined by the P value results for this soil; in only one case out of 9 was the P value <90% (Table 1). In comparison, the other methods resulted in 6, 4, 7, and 2 tests out of 9 with P value lower than 90% for the LIN-2, ML-2, ML-3, and NLIN-2 methods, respectively. The ML-3 method gave significantly higher ($P < 0.05$) D values than the other methods, and the corresponding P values were lower than 70% in 5 out of 9 cases. Further, the ML-3 method displayed highest AIC estimate (Table 2).

Parameter Estimates

The method used to estimate the Weibull parameters had a significant effect ($P < 0.05$) on both the characteristic strength, α, the spread of strengths, β, and the location parameter, E_0 (Table 3). For the Bygholm and Maury soils, the ML-2 and LIN-2 methods gave significantly higher α values than the other methods. The ML-3 method produced significantly lower α values for the Maury and Karnak soils. Significantly higher estimates of β were produced when this parameter was estimated for the two-parameter model. The ML-3 method resulted in significantly lower β estimates. For E_0, the ML-3 method produced significantly higher estimates than the NLIN-3 method for the Maury and Karnak soils; there was no significant difference between these methods for the Bygholm soil.

Table 2. Mean AIC estimates for the different models and estimation methods.

		AIC †			
Soil	n	NLIN-2	ML-2	NLIN-3	ML-3
Bygholm	8	−299 b‡	−279 b	−322 c	−236 a
Maury	36	−270 c	−252 b	−275 c	−221 a
Karnak	9	−276 b	−263 b	−278 b	−221 a

† NLIN-2 = nonlinear regression, two-parameter Weibull model; ML-2 = maximum likelihood, two-parameter Weibull model; NLIN-3 = nonlinear regression, three-parameter Weibull model; ML-3 = maximum likelihood, three-parameter Weibull model.
‡ Means with the same letter within a site are not significantly different at $P < 0.05$ according to a t test.

Correlations were performed between the parameter estimates from each method across all soils, treatments, and size fractions. The estimated α values generated by the different methods were strongly positively correlated ($R^2 \geq 0.99$) in all cases. Much weaker correlations were generally observed for the β parameter (Table 4), although estimates from the LIN-2, NLIN-2, and ML-2 methods showed rather strong relationships ($R^2 = 0.67$–0.80).

Parameter Sensitivity to Soils, Management, and Sizes

For such E datasets, the main objective is usually to investigate soil, treatment, and size effects. Regardless of estimation method, the α parameter clearly indicated that aggregate strength was lowest for the Bygholm sand loam, intermediate for the Maury silt loam, and highest for the Karnak silty clay.

For the comprehensive Maury dataset, it was possible

Table 3. Model and estimation method effects on characteristic strength, α, spread of strength, β, and strength at zero probability of failure, E_0.

		Method†				
Soil	Parameter	LIN-2	NLIN-2	ML-2	NLIN-3	ML-3
Bygholm	α (J/kg)	3.77‡ a§	3.56 b	3.77 a	3.53 b	3.55 b
n = 8	β	1.82 a	1.87 a	1.73 b	1.45 c	1.34 d
	E_0 (J/kg)	n.d.¶	n.d.	n.d.	0.62 a	0.65 a
Maury	α (J/kg)	7.90 a	7.61 b	7.87 a	7.56 b	7.39 c
n = 36	β	1.49 a	1.48 a	1.48 a	1.30 b	1.19 c
	E_0 (J/kg)	n.d.	n.d.	n.d.	0.56 b	0.80 a
Karnak	α (J/kg)	14.85 a	14.67 a	14.66 a	14.61 a	13.75 b
n = 9	β	1.40 ab	1.44 a	1.49 a	1.35 b	1.18 c
	E_0 (J/kg)	n.d.	n.d.	n.d.	0.56 b	1.26 a

† LIN-2 = linear regression, two-parameter Weibull model; NLIN-2 = nonlinear regression, two-parameter Weibull model; ML-2 = maximum likelihood, two-parameter Weibull model; NLIN-3 = nonlinear regression, three-parameter Weibull model; ML-3 = maximum likelihood, three-parameter Weibull model.
‡ Values are least square means across treatments and sizes within each site.
§ Means with the same letter within a row are not significantly different at $P < 0.05$ according to a t test.
¶ Not determined for the 2-parameter model.

Table 4. Coefficients of determination, R^2, between β estimates from the different model/estimation methods.†

	LIN-2	NLIN-2	ML-2	NLIN-3	ML-3
NLIN-2	0.76***‡				
ML-2	0.80***	0.67***			
NLIN-3	0.17**	0.54***	0.28***		
ML-3	0.16**	0.30***	0.31***	0.39***	

** Significant at $P < 0.01$.
*** Significant at $P < 0.001$.
† LIN-2 = linear regression, two-parameter Weibull model; NLIN-2 = nonlinear regression, two-parameter Weibull model; ML-2 = maximum likelihood, two-parameter Weibull model; NLIN-3 = nonlinear regression, three-parameter Weibull model; ML-3 = maximum likelihood, three-parameter Weibull model.
‡ Correlations carried out across soils, treatments, and sizes.

to evaluate the power of discrimination between tillage treatments and size classes for the different methods on a given soil. Perfect et al. (1998) showed that there was significant effect of tillage and size on α when this parameter was estimated using NLIN-2. In this study, highly significant ($P << 0.05$) F-values were obtained for both tillage and size effects on α, irrespective of the estimation method. The interaction between tillage and size was not significant at $P < 0.05$ in all cases. The power of distinction between treatments (i.e., the F-values produced by the ANOVA) was highest for the NLIN methods and lowest for the ML-3 method (Fig. 2).

In terms of β, Perfect et al. (1998) found a significant effect of size but not of tillage when this parameter was estimated by the NLIN-2 method for the Maury data set. In this study there was no significant tillage effect on β whatever model/estimation method was used to estimate β (data not shown). An effect of size on β was found for all two-parameter model estimation methods, but not for the three-parameter model irrespective of estimation method (data not shown).

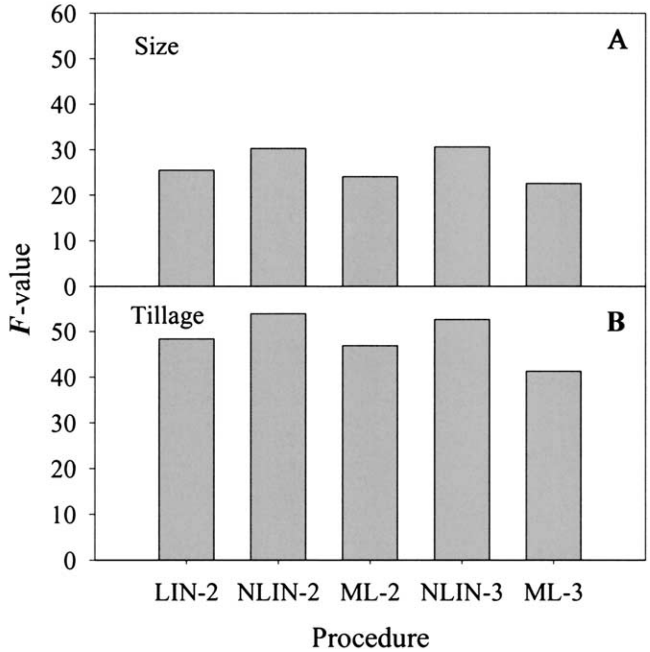

Fig. 2. F-values for effect of (A) treatment and (B) size determined in analysis of variance for the α parameter estimated by the different methods for the Maury soil. LIN-2 = linear regression, two-parameter Weibull model; NLIN-2 = nonlinear regression, two-parameter Weibull model; ML-2 = maximum likelihood, two-parameter Weibull model; NLIN-3 = nonlinear regression, three-parameter Weibull model; ML-3 = maximum likelihood, three-parameter Weibull model.

DISCUSSION

The P-values for the predicted distributions suggest that adding an extra parameter improved fitting using the NLIN method. The NLIN-3 method gave a significantly lower (more negative) mean AIC value relative to the NLIN-2 method for the Bygholm but not for the Maury and Karnak soils (Table 2). The power of distinction between treatments on the Maury soil was not improved by using the three-parameter model instead of the two-parameter model (Fig. 2).

The choice of model/estimation method had a significant effect on the parameter values. This implies that the type of model should be taken into account when comparing α and β values across studies. We found significantly lower estimates of β for the three- versus the two-parameter model. Trustrom and Jayatilaka (1979) showed that E_0 and β were strongly correlated, since the estimate of β decreased systematically when increasing E_0 for a simulated dataset.

In our study the NLIN method outperformed both the LIN and ML methods. The NLIN method produced clearly better goodness-of-fits across sites, and gave higher F-values for tillage and size effects on α for the Maury soil. The traditionally used LIN method performed rather poorly in this study, which was not surprising. Even though the method is simple and easy to work with, it may have some profound shortcomings. Often double log-transformed Weibull plots show a lack of straight line fit (Perfect et al., 1998), which was also found in this study in most cases (data not shown). Diverging extreme low or high values have a much stronger effect on parameter estimates when using the LIN as compared with the NLIN method. Such diverging values are common for soil brittle fracture data and Braunack et al. (1979) suggested omitting the first and the last two points in the LIN-2 fitting. They assumed that the extreme values were outliers. This approach of systematically omitting extreme values is not good practice since valuable information may be lost.

The poor performance of the ML method was surprising since this method is considered a more accurate and robust method than the LIN method (Seguro and Lambert, 2000; Lawless, 2003) for estimating parameters in the two-parameter Weibull model. For simulated datasets, the ML method has provided less biased parameter estimates and lower standard errors of estimates than those produced by the LIN method for a two-parameter Weibull model (Trustrom and Jayatilaka, 1979). However, the ML method was not better than the LIN method when sample numbers were small ($n < 30$) (Trustrom and Jayatilaka, 1979; Khalili and Kromp, 1991; Clarke, 2003). The rather poor performance of ML-2 in this study, in comparison with NLIN-2, may be due to the fact that sample numbers were relatively small (i.e., $n = 40$ or 45), as is common in soil studies. For ML estimation, inclusion of a third parameter in the Weibull model improved the goodness-of-fit for the Bygholm soil, but not for the Maury and Karnak soils (Fig. 1). In fact, the ML-3 method produced a lower goodness-of-fit compared with the ML-2 method for the Karnak soil.

The poor performance of the ML-3 method, especially for the Maury and Karnak soils, may be due to an unexpected methodological problem. The likelihood function is unbounded for $\beta < 1$ and there is no global maximum to the likelihood equation, Eq. [5] (Lawless, 2003). In our study, $\beta < 1$ occurred in 1 out 8, 12 out 36, and 5 out of 9 of the ML-3 fits for the Bygholm, Maury and Karnak soils, respectively. As a result, it may be argued that statistical comparison of ML-3 with the other methods was not strictly valid. However, the occurrence of β values < 1 was not expected beforehand (Perfect and Kay, 1994). Clearly, this problem limits the applicability of the ML-3 method for fitting soil brittle fracture data.

Our results showed that the α and β parameters were markedly dependent on the estimation method. In particular, the ML-3 method resulted in apparently biased values of α and β, which may be related to the previously mentioned methodological problem. However, significant differences were also found between the other methods. Therefore, comparisons across studies with different estimation methods must be done with caution. We found a very strong correlation between values of α estimated by the different methods. This means that α for a given estimation method can be estimated from the α estimated by a different method. For β the situation is more complex. Rather strong correlations ($R^2 > 0.67$) were found between estimates from the two-parameter model and between NLIN-2 and NLIN-3 (Table 4). Weaker correlations were found between estimates from the two different model types as well as between the three-parameter model estimation methods. The reciprocal of β has been used as an estimate of soil friability with fixed threshold values (Perfect and Kay, 1994). Our findings highlight the importance of using a standard method for estimating β to be able to make comparisons across studies.

CONCLUSIONS

In this study we evaluated the use of two- and three-parameter Weibull distributions to model brittle fracture of air-dry soil aggregates. We found that a three-parameter model in most cases resulted in slightly better goodness-of-fit than a two-parameter model when the parameters were estimated using nonlinear regression. However, a three-parameter model did not significantly improve the power of discrimination between management treatments and aggregate size for the Maury soil (the only site that permitted such an analysis). The estimates of characteristic strength, α, and spread of rupture energies, β, significantly depended on model type as well as on the estimation method used. A three-parameter model produced lower estimates of β than a two-parameter model. The data were best-fitted using nonlinear regression. Nonlinear regression also resulted in a greater power of distinction between tillage treatments and size fractions for α on the Maury soil.

Even though the three-parameter Weibull model resulted in the best overall goodness-of-fit, we recommend that aggregate rupture data continue to be fitted to the simpler two-parameter Weibull model provided the parameters are estimated using nonlinear regression. With this method there was only a small difference in goodness-of-fit between the two- and three-parameter Weibull models. Our results suggest that use of a two-parameter model, with nonlinear regression estimation of parameters, increases the goodness-of-fit and improves the ability to discriminate between treatments in comparison with the traditional linear regression estimation method. In addition, the continued use of a two-parameter Weibull model will make it easier to compare future results with those already published in previous studies.

ACKNOWLEDGMENTS

The technical assistance of B.B. Christensen and Q. Zhai is gratefully acknowledged. The Danish Agricultural and Veterinary Research Council financed most of this work.

REFERENCES

Braunack, M.V., J.S. Hewitt, and A.R. Dexter. 1979. Brittle fracture of soil aggregates and the compaction of aggregate beds. J. Soil Sci. 30:653–667.

Clarke, R.T. 2003. Comparison of estimators of linear time trend in Weibull-distributed low flows. Water Res. Res. 39:doi10.1029/2002WR001640.

Dexter, A.R., and C.W. Watts. 2000. Tensile strength and friability. p. 405–433. *In* K.A. Smith and C.E. Mullins (ed.) Soil and environmental analysis physical methods. Marcel Dekker Inc., New York.

Ferreira, J.L.A., J.C. Balthazar, and A.P.N. Araujo. 2003. An investigation of rail bearing reliability under real conditions of use. Eng. Failure Anal. 10:745–758.

Frantziskonis, G. 1995. Heterogeneity and implicated surface effects: Statistical, fractal formulation and relevant analytical solution. Acta Mech. 108:157–178.

Freudenthal, A.M. 1968. Statistical approach to brittle fracture. p. 591–619. *In* H. Liebowitz (ed.) Fracture: An advanced treatise. Vol. II. Mathematical fundamentals. Academic Press, New York.

Herrmann, H.J., and S. Roux (ed.). 1990. Statistical models for the fracture of disordered media. North-Holland, Amsterdam, The Netherlands.

Khalili, A., and K. Kromp. 1991. Statistical properties of Weibull estimators. J. Mat. Sci. 26:6741–6752.

Lawless, J.F. 2003. Statistical models and methods for lifetime data. John Wiley & Sons, Hoboken, NJ.

Mahdi, S., and F. Ashkar. 2004. Exploring generalized probability weighted moments, generalized moments and maximum likelihood estimating methods in two-parameter Weibull model. J. Hydrology 285:62–75.

Munkholm, L.J., and B.D. Kay. 2002. Effect of water regime on aggregate tensile strength, rupture energy and friability. Soil Sci. Soc. Am. J. 66:702–709.

Munkholm, L.J., and P. Schjønning. 2004. Structural vulnerability of a sandy loam exposed to intensive tillage and traffic in wet conditions. Soil Tillage Res. 79:79–85.

Perfect, E., and B.D. Kay. 1994. Statistical characterization of dry aggregate strength using rupture energy. Soil Sci. Soc. Am. J. 58: 1804–1809.

Perfect, E., and B.D. Kay. 1995. Brittle fracture of fractal cubic aggregates. Soil Sci. Soc. Am. J. 59:969–974.

Perfect, E., Q. Zhai, and R.L. Blevins. 1997. Soil and tillage effects on the characteristic size and shape of aggregates. Soil Sci. Soc. Am. J. 61:1459–1465.

Perfect, E., and R.L. Blevins. 1997. Fractal characterization of soil aggregation and fragmentation as influenced by tillage treatment. Soil Sci. Soc. Am. J. 61:896–900.

Perfect, E., Q. Zhai, and R.L. Blevins. 1998. Estimation of Weibull brittle fracture parameters for heterogeneous materials. Soil Sci. Soc. Am. J. 62:1212–1219.

SAS Institute. 1999. SAS OnlineDoc V8. SAS Inst. Cary, NC.

Seguro, J.V., and T.W. Lambert. 2000. Modern estimation of the parameters of the Weibull wind speed distribution for wind energy analysis. J. Wind Eng. Ind Aerod 85:75–84.

Shih, T.T. 1980. An evaluation of the probalistic approach to brittle design. Eng. Fract. Mech. 13:257–271.

Srolovitz, D.J., and P.D. Beale. 1988. Computer simulation of failure in an elastic model with randomly distributed defects. J. Am. Ceram. Soc. 71:362–369.

Trustrum, K., and A.d.S. Jayatilaka. 1979. On estimating the Weibull modulus for a brittle material. J. Mat. Sci. 14: 1080–1084.

Utomo, W.H., and A.R. Dexter. 1981. Soil friability. J. Soil Sci. 32: 203–213.

Weibull, W. 1952. A survey of “statistical effects” in the field of material failure. Appl. Mech. Rev. 5:449–451.