Representing Aggregate Size Distributions as Modified Lognormal Distributions

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Abstract. *Historically, the two-parameter lognormal distribution has been the method of choice when describing soil aggregate size distributions and generally provides a good description. However, the assumptions regarding the upper and lower extremes of the two-parameter lognormal ogive can limit its applicability to many tillage-induced aggregate size distributions. Two 3-parameter and one 4-parameter lognormal ogives are presented that can more accurately describe a wider range of field-sampled aggregate size distributions. Two computational techniques for determining values for the coefficients of these modified lognormal functions are discussed. One is a direct computation method, useful for applications where computation speed is a factor. The second method uses a nonlinear optimization technique, which will find the "best fit" parameter values more precisely, but requires more computational overhead.*
Keywords. *Aggregate size distribution, Lognormal distribution, Curve-fitting, Frequency distribution.*

The size distribution of soil aggregates affects many facets of agriculture from wind erosion susceptibility (Chepil, 1950a, 1953) to seedbed suitability (Hadas and Russo, 1974; Schneider and Gupta, 1985). Gardner (1956) demonstrated that the two-parameter lognormal distribution provided a good description of the mass-based aggregate size distribution (ASD) of many soils. Kemper and Chepil (1965) concurred with Gardner, extolling the virtue of summarizing ASD data with only the two parameters, geometric mean diameter, x_g, and geometric standard deviation, σ_g. Unfortunately, they did not recommend this method for general use because of the extensive work required to adequately sieve field samples and the computational effort required to determine the parameters. This led to the adoption of many less meaningful measures of ASD. For this reason, Hagen et al. (1987) presented a computerized iteration procedure that required only two sieves to determine the parameters for a standard, two-parameter lognormal ogive to characterize ASD of dry soil. The one caveat that Gardner mentioned is that any field-sampled, ASD will exhibit some deviation at the extremes from a standard lognormal ogive. Hagen et al. (1987), also realizing this limitation, suggested the possibility of using three- or four-parameter lognormal forms if the tails of the distributions are important to the application of the data.

Knowing the complete ASD provides useful information about wind erosion processes. Examples follow:

- Given different ASDs with the same percentage of erodible aggregates (less than 0.84 mm), Chepil (1950b) showed that ASDs with smaller nonerodible aggregates resulted in more rapid surface armoring and, thus, a less erodible fraction available for direct emission. Thus, many small nonerodible aggregates provide more surface cover and shelter for the erodible soil than do a few large non-erodible aggregates. Therefore, with a complete ASD, it is possible to determine the amount of "shelter" provided by nonerodible aggregates (Wagner and Hagen, 1991).
- Given a complete ASD and a shelter angle distribution (Potter et al., 1990) and assuming that the smallest aggregates are residing in the most sheltered areas, we can:
    - compute the fraction of soil surface where friction velocity is above saltation threshold
    - compute the volume of particles available for emission (Hagen, 1991)
    - estimate the fraction of PM-10 (sub 10-μm-size particles) present for direct emission [PM-10 has health and regulatory implications (Stonefield, 1988; Barnard et al., 1992)]
- With a complete ASD, the effect of sorting by wind erosion can be determined. Size ranges for saltation, suspension, and emission materials change with windspeed and surface roughness. Therefore, these components can be studied together in relation to surface ASDs obtained following wind erosion events.

Knowing the complete ASD is also important to modeling tillage processes. Many tillage-induced ASDs are influenced by the amount and size of the largest aggregates in the field prior to tillage. Wagner and Ding (1993)

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showed that disk tillage operations primarily break down large aggregates (greater than 50 mm) when they are present, but reduce a wide range of aggregate sizes when large aggregates do not exist. Therefore, the resulting post-tillage ASD is dependent upon the pre-tillage ASD. Future advances in modeling aggregate breakdown by tillage operations will necessarily require accurate representation of the pre-tillage ASD.

The Wind Erosion Prediction System (WEPS), presently being developed by the USDA-Agricultural Research Service (Hagen, 1991), requires the dry ASD to be accurately represented on a daily basis within the model. The standard lognormal ogive implies that the smallest aggregate size is zero and the largest size is infinite. Agricultural soils however have upper and lower size limits, which account for ASD deviations from lognormality. These deviations become more pronounced when sorted into additional size classes to more accurately estimate the "true" ASD. For these reasons, a more complete method of representing ASD was desired for WEPS.

Kottler (1950a), Irani (1959), and Irani and Callis (1963) examined situations that arose when data conforming to lognormality had all sizes greater than or less than a specified size (or both) removed from the data set. The modified data sets were actually similar to many of the data sets typically presented as being lognormal distributions. In these "nonideal" cases, physical constraints limit the "growth" or "breakdown" process, and, therefore, were not truly lognormal. They showed that the "limited growth" and "limited breakdown" processes could still easily be represented by a lognormal ogive when simple transformations were applied that satisfied the new boundary conditions.

By introducing these two, potentially physically based parameters, a transformation can be established between the real distribution of the data and the standard lognormal distribution, resulting in a modified lognormal distribution. Since all dry ASDs have some physical limiting maximum and minimum sizes, modified lognormal ogives should presumably be more accurate in representing entire ASD distributions. The purpose of this article is to describe the procedures required to determine the parameters of the modified lognormal ogive and present methods for computing their values. Comparisons between the standard and modified lognormal ogives were made using actual ASDs determined from sieved field samples.

THEORY

Particle sizes, such as soil aggregate sizes, are frequently found empirically to fit the lognormal distribution function. If x is the quantity being measured and is to be described by a lognormal distribution, then $y = \ln(x)$ has a normal distribution n(y) (eq. 1), in which the parameters μ and σ^2 are respectively, the mean and the variance of the y values. Because n(y) is symmetric about the mean, μ is also the median of the normal distribution (on the average, half the y values will be greater than μ and half will be less). Since x is the quantity being measured (e.g., aggregate size), it will be found to be distributed with a density function, p(x), where p(x)dx is the probability that a measured value will fall within the range [x, x + dx]. Because p(x) and n(y) describe the same phenomenon, the probability of obtaining values in corresponding dy and dx intervals must be equal, i.e., $p(x)dx = n(y)dy$. Thus, the lognormal distribution p(x) is given by equation 2.

$$n(y) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(y-\mu)^2}{2\sigma^2}\right] \quad -\infty < y < +\infty \tag{1}$$

$$p(x) = n(y)\frac{dy}{dx} = \frac{1}{x\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(\ln(x)-\mu)^2}{2\sigma^2}\right] \quad 0 < x < +\infty \tag{2}$$

The average value of x is defined as:

$$x_{av} \equiv \int_0^{\infty} x\, p(x)\, dx = \int_{-\infty}^{\infty} e^y n(y)\, dy \tag{3}$$

Because $y = \ln(x)$, we have the median value, $x_m = \exp(\mu)$. By substituting this and equation 2 into equation 3 and integrating we have $x_{av} = \exp(\mu+\sigma^2/2)$. For a lognormal distribution, σ^2 is always larger than zero; thus, the lognormal distribution can be fully described by the median size, x_m, and the mean size, x_{av}. In other words, from the observed mean and median, values for μ and σ^2 of the approximating lognormal distribution can be estimated as $\mu = \ln(x_m)$ and $\sigma^2 = 2[\ln(x_{av})-\mu] = 2[\ln(x_{av})-\ln(x_m)]$.

However, most lognormal distributions are expressed in terms of the geometric mean, x_g, and geometric standard deviation, σ_g, which are defined as $x_g \equiv \exp(\mu)$ and $\sigma_g \equiv \exp(\sigma)$, respectively. Substituting x_g and σ_g into equation 2, p(x) can be expressed in terms of x_g and σ_g. For many analyses, it is often useful to express the measured distribution in terms of the cumulative probability distribution, F(x), which is the probability (or frequency) that a measured value will be less than or equal to x. If $t \equiv \ln(x/x_g)/\ln(\sigma_g)$, then for the lognormal distribution, this cumulative distribution function of x is given by:

$$F(x) \equiv \int_0^{x} p(x)\, dx = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{t} e^{-t^2/2}\, dt = \frac{1}{2} + \frac{1}{2}\operatorname{erf}\left(\frac{t}{\sqrt{2}}\right) = \frac{1}{2} + \frac{1}{2}\operatorname{erf}\left(\frac{\ln(x)-\ln(x_g)}{\sqrt{2}\,\ln(\sigma_g)}\right) \tag{4}$$

Thus, the probability of x, $P(\% \le x)$ and $P(\% \ge x)$, in terms of percent, can be calculated as:

$$P(\% \le x) = 100F(x) = 50 + 50\operatorname{erf}\left(\frac{\ln(x)-\ln(x_g)}{\sqrt{2}\,\ln(\sigma_g)}\right),$$

$$P(\% \ge x) = 100 - P(\% \le x) \tag{5}$$

Kottler (1950a) treated particle size distributions from a kinetic point of view. He discussed the concept of "limited growth" in which most phenomena of normal growth have a rate that increases only during an initial period and afterwards decreases gradually. He introduced a lower limit, x_0 (corresponding to the absolute minimum particle size), which must be greater than zero and an upper limit, x_∞ (corresponding to the absolute maximum size obtained), which must be less than infinity. By using the transformation, $x' = (x - x_0)(x_\infty - x_0)/(x_\infty - x)$ in which x is in the range of $[x_0, x_\infty]$, where $0 \le x_0 < x_\infty < +\infty$, a more general four-parameter lognormal case, equation 6, can be introduced.

$$p(x') = \frac{1}{x'\sqrt{2\pi}\,\ln(\sigma'_g)} \exp\left[-\frac{1}{2}\left(\frac{\ln(x'/x'_g)}{\ln(\sigma'_g)}\right)^2\right]$$

$$0 < x' < +\infty \qquad (6)$$

The corresponding cumulative distribution function, in terms of percent, are:

$$P'(\% \le x) = 50\left\{1 + \mathrm{erf}\left[\frac{\ln\left(\frac{(x - x_0)(x_\infty - x_0)}{(x_\infty - x)\,x'_g}\right)}{\sqrt{2}\,\ln(\sigma'_g)}\right]\right\},$$

$$P'(\% \ge x) = 100 - P'(\% \le x) \qquad (7)$$

Both x'_g and σ'_g can be determined from computational procedures discussed later. To obtain the x_g value from x'_g, simply perform the reverse transformation operation of x' as shown in equation 8. Note that x_g is the 50% value, x_{50}, and represents the "middle" of the distribution.

$$x_g \equiv x_{50} = \frac{x'_g x_\infty + x_0 x_\infty - x_0^2}{x_\infty - x_0 + x'_g} \qquad (8)$$

To obtain the σ_g value from σ'_g, compute the arithmetic average of the x' values, x'_{av}:

$$x'_{av} = x'_g \exp\left[1/2 \ln^2(\sigma'_g)\right] \qquad (9)$$

to obtain x_{av}, perform the transformation as shown in equation 10 on x'_{av}:

$$x_{av} = \frac{x'_{av} x_\infty + x_0 x_\infty - x_0^2}{x_\infty - x_0 + x'_{av}} \qquad (10)$$

and then compute σ_g as a function of x_{av} and x_g as shown in equation 11.

$$\sigma_g = \exp\left[\sqrt{2}\,\ln^{1/2}\left(\frac{x_{av}}{x_g}\right)\right] \qquad (11)$$

If $x_0 = 0$ and $x_\infty \to \infty$, this general case, equation 6, will reduce to the simple or standard, two-parameter lognormal distribution, equation 2, and its corresponding cumulative distribution function, equation 5. Either of the three-parameter forms are derived when the lower value, x_0, equals zero or the upper value, x_0, approaches infinity. All of these lognormal forms are summarized in table 1.

Computational Procedures

Two methods of computing the parameters for the four forms of the lognormal ogives discussed here were implemented. One method uses a direct computational scheme, and the second employs a nonlinear optimization technique to determine the "best" parameters based on the cumulative distribution curve.

The direct computational scheme outlined by Allen (1981) and Campbell (1985) uses the assumption that the data are lognormally distributed and works best when the sieve cuts are sized according to a geometric progression. It requires an estimate of the minimum size, x_{min}, and the maximum size, x_{max}, (to determine the geometric means, $x_{g(0)}$ and $x_{g(n)}$, of the smallest and largest sieve cuts respectively). Also, if a modified lognormal form is being used, the additional constraints must also be followed: $x_{min} < x_0 < x_{g(0)}$, and $x_{g(n)} < x_\infty < x_{max}$.

The disadvantages of this method are that:

- An estimate of the geometric means of the smallest and largest sieve cuts must be made.
- The limits of the distribution, x_0 and x_∞, must be known (or their ranges known if an optimization technique is employed to determine them).
- Due to the constraints on x_0 and x_∞, if the smallest and/or largest sieve cuts have no material in them for a particular distribution, they must be removed from the computations if the limiting parameters, x_0 and/or x_∞, need to fall within those size ranges.

The benefit of the direct computational scheme is that it is very fast and does not require any iterative procedures, making it suited for applications where speed is critical.

For the direct computational procedure, the estimated (or sample) geometric mean diameter, x'_g, and geometric standard deviation, σ'_g, are:

$$x'_g = e^a \text{ and } \sigma'_g = e^b \qquad (12)$$

where

$$a = \sum_{i=1}^{n}\left[m_i \ln(x'_{g(i)})\right]$$

$$b = \left[\sum_{i=1}^{n}\left[m_i \ln^2(x'_{g(i)})\right] - a^2\right]^{\frac{1}{2}}$$

i = sieve cut

$x'_{g(i)} = \sqrt{x'_{i(lower)}\, x'_{i(upper)}}$ = geometric mean within sieve cut i

n = total number of sieve cuts

m_i = mass fraction of sieve cut i

Table 1. Standard and modified lognormal forms

Case	Log-normal Form	Constraints	Parameters
I	standard 2-parameter	$0 \le x < \infty$	x_g, σ_g
II	modified 3-parameter	$0 \le x \le x_\infty < \infty$	$x'_g, \sigma'_g, x_\infty$
III	modified 3-parameter	$0 < x_0 \le x < \infty$	x'_g, σ'_g, x_0
IV	modified 4-parameter	$0 < x_0 \le x \le x_\infty < \infty$	$x'_g, \sigma'_g, x_0, x_\infty$

The second method uses a constrained optimization procedure to estimate the parameters of the cumulative frequency curve for any of the selected lognormal forms (equation 6). We chose to use forms of the downhill simplex method in multidimensions (Press, et al., 1986). The function used to determine the "best fit" was the weighted sum of the squared residuals due to error (SSE) as shown in equation 13.

$$SSE = \sum_{i=1}^{n} \left[w_i \left(\hat{y}_i - y_i \right)^2 \right] \qquad (13)$$

where

- i = data value
- n = total number of data values
- x_i = sieve size for data value i
- y_i = actual P′ (% ≤ x_i)
- $\hat{y}_i$ = estimate of P′ (% ≤ x_i)
- w_i = weighting factor for data value i

The actual and predicted probabilities less than (or greater than) the sieved sizes were used as the y values. Kottler (1950b) suggested that "fitting" lognormal data should generally employ a probability weighting factor if the 50% point is of greatest interest. Kottler went on to explain that these weighted least squares, Mueller Weights, are required for curve-fitting to a standard lognormal ogive to compensate for the exaggerations due to the probability scale on a Probability Graph, which is actually a t-scale and not a P-scale. Additional weighting schemes may also be employed depending upon the region of interest, type of data, and experimental errors encountered. However, when working with the modified lognormal forms, the curve-fit errors usually associated with the tails of the distribution are reduced sufficiently that a unit weighting factor is usually adequate for the modified lognormal forms.

The limitation of the method is that it is an iterative procedure and, therefore, may not be appropriate for use in applications where speed is critical. Nevertheless, it will determine the "best fit" without the limitations and assumptions required of the direct computation procedure. It does need estimates of the upper and lower ranges for each of the parameters being determined. These can be set broadly enough to encompass all expected size distributions. Narrower ranges, if known, will allow the optimization procedure to "close in" on the solution faster, but are not strictly required. By setting the upper and lower ranges equally for a particular parameter, then the optimization routine would effectively force the "best fit" model to have the desired value for that parameter.

Since computational complexity was cited as one of the reasons for lognormal distributions not being universally adopted as a measure of soil ASD (Hagen et al., 1987), despite the advantages listed by Gardner (1956), a computer program, code-named "asd", was written to assist in the model parameter identification process*. The "asd" program is written in the C language, contains both a command-line and a menu-based user interface, and can display the results graphically onscreen for visual feedback on the "goodness of fit". The program can run under either DOS or the UNIX operating system. The main functions available to the user are: executing the curve fit analysis routine, viewing the output either numerically or graphically on the screen or to a printer, selecting the curve-fit analysis choices and options, and creating a default configuration file.

The ASD data sets presented as examples were obtained on a range of soils from several experimental field studies, some of which have been published (Tangie et al., 1990; Ambe, 1991; and Wagner et al., 1992), under a variety of aggregate formation conditions. ASD samples (approximately 10 kg) were collected from the first 15 cm or from within the tillage tool processing depth if a post-tillage sample. The samples were extracted using a 30 × 23 cm flat, square-cornered shovel, as described by Chepil (1962), and placed in 46 × 30 × 6 cm plastic tubs. All ASD samples were air-dried in a greenhouse prior to sieving with a modified combined rotary sieve (Lyles et al., 1970). Some of the ASD sets also had the smallest size class obtained from the rotary sieve (< 0.42 cm) sieved into smaller size classes with a sonic sieve.

Discussion

Because the field ASDs physically have lower and upper size limits, the four-parameter, modified lognormal function is recommended for describing the distribution. If only one of the distribution tails is of interest or there is insufficient sampling within one of the tail regions, selection of the appropriate three-parameter, modified lognormal function may be adequate. If only the geometric mean size of the distribution is of interest, then a standard lognormal function determined with Mueller weights may suffice.

The standard, two-parameter lognormal distribution is completely described by x_g and σ_g. By definition, the geometric mean, x_g, for the two-parameter lognormal function directly provides the size at which 50% is greater and 50% is less than its value. The geometric standard deviation, σ_g, is defined as the ratio of the size at 84.13% probability to the size at 50% probability (or the size at 50% probability to the size at 15.87% probability) and indicates the dispersion or range of sizes for a two-parameter lognormal function.

The addition of new parameters for the modified lognormal functions allow more accurate descriptions of typical size distributions, but makes comparisons of such size distributions more difficult. Both x'_g and σ'_g parameters represent the physical relationships mentioned above, but they apply to the transformed variable, x′, and not to the original variable, x, for the modified lognormal functions. Both x'_g and σ'_g are defined in terms of the

* Code employing the computational methods discussed are available upon request by sending a DOS compatible disk to the primary author.

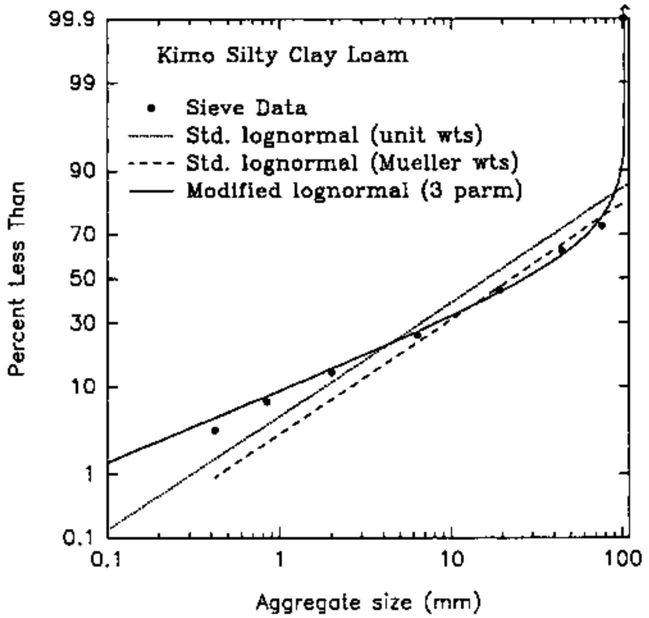

Figure 1–ASD sample showing effects of Mueller weighting on a standard lognormal fit and benefits of the modified lognormal.

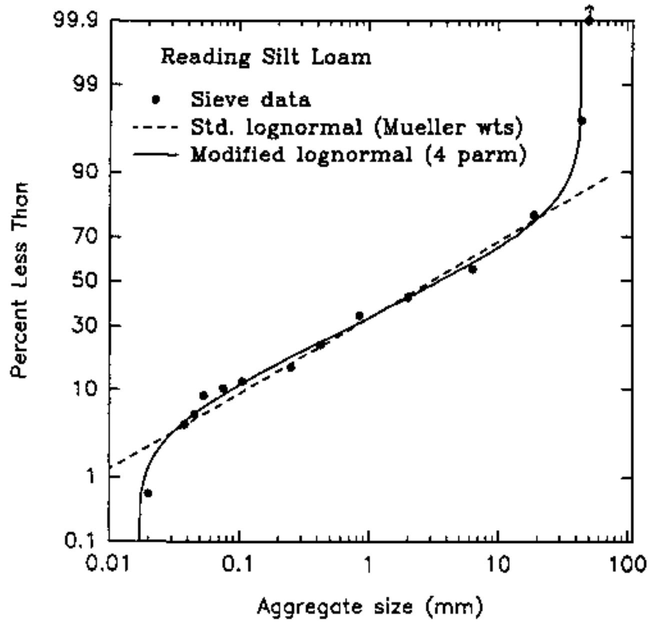

Figure 2–ASD sample showing a four-parameter modified lognormal fit to the data.

transformation variable, x', and are functions of the x_0 and x_∞ parameters. Therefore, the x'_g and σ'_g terms (table 1) for the modified lognormal functions are not directly comparable with each other or with x_g and σ_g terms from the standard lognormal function. Thus, care must be taken not to make comparisons and draw conclusions based solely on the modified lognormal parameters, x'_g and σ'_g, if the lower and upper limits, x_0 and x_∞, are not the same.

Ropp (1985) discussed this problem along with the tendency of many researchers to assume normality or even lognormality and then present only the fraction of interest. He suggested that the most effective method for displaying ASDs is to use a lognormal probability method. Because no one parameter or group of parameters can be defined for use when presenting and discussing all size distribution information, visual presentation of the data, and summarization of the parameters describing the complete distribution are requisite, especially when using one of the modified lognormal forms.

The effectiveness of using modified lognormal distributions are illustrated in the following examples. Figure 1 is a post-tillage ASD from a Kimo silty clay loam (clayey over loamy, mesic Fluvaquentic Montmorillonitic) in which a very high percentage of large aggregates were formed from a chiseling operation. Figure 1 shows the benefit of Mueller weights over unit weights on the estimation of x_g when using the standard two-parameter lognormal form. However, Mueller weighting does not necessarily improve the "fit" of a standard lognormal form to the full distribution as represented by this data set. A three-parameter, modified lognormal fit is also presented to show how it can better represent the full distribution, including the upper 30% of the ASD than the standard lognormal form with or without Mueller weighting.

Figure 2 is an ASD from a Reading silt loam (fine-silty, mixed, mesic Typic Argiudoll) that had the smaller fraction sieved into additional size classes to more accurately determine the form of the lower tail of the distribution. Notice that this distribution also reflects a large amount of big aggregates that causes the cumulative distribution to deviate from a straight line in the upper 30% of the distribution similar to the ASD in figure 1. The four-parameter lognormal form fit this distribution very well and determined the lower limit, x_0, to be 0.16 mm and the upper limit, x_∞, to be 45.9 mm (table 2). Due to the additional sieve cut data at the lower end of the distribution, it partially compensates the effect of the deviation from a lognormal distribution at the high end. Thus, the standard lognormal fit using Mueller weights does a fair job of representing the "middle" of this particular ASD. However, it does not represent either of the tails accurately.

Table 2. Standard and modified lognormal coefficients for several aggregate size distributions

Soil	Log-normal Form	Weights	x_{50}	σ_g	Std Dev	Wt r^2	x'_g	σ'_g	x_0	x_∞
Kimo	2-parameter	Unit	19.85	5.38	2.512	0.952	19.85	5.38	-	-
	2-parameter	Mueller	22.44	5.38	0.471	0.984	22.44	5.38	-	-
	3-parameter	Mueller	26.84	5.07	0.222	0.996	35.63	14.60	-	108.8
Reading	2-parameter	Mueller	3.03	13.06	0.237	0.995	3.03	13.06	-	-
	4-parameter	Unit	3.48	9.28	0.428	0.998	3.74	22.06	0.016	45.9
Keith	3-parameter	Unit	12.39	6.38	1.240	0.989	14.52	12.79	-	84.75
Ulysses	3-parameter	Unit	0.96	14.47	0.454	0.997	0.98	22.21	-	47.65

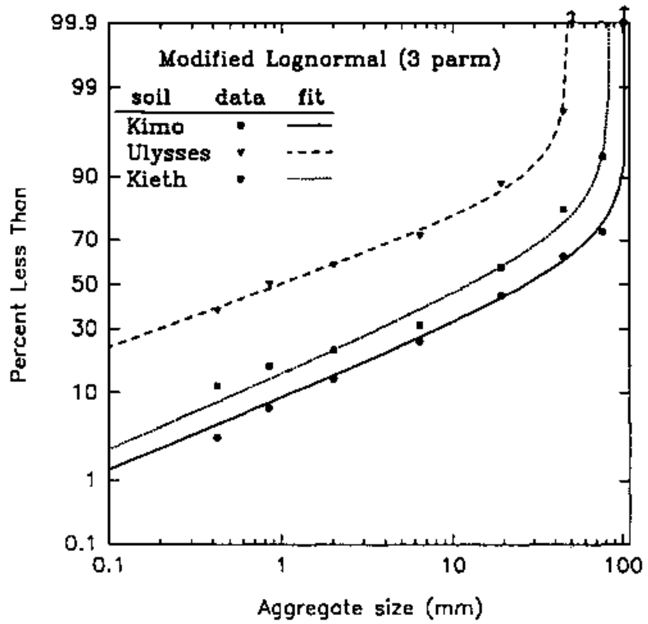

Figure 3–Various ASD samples showing a three-parameter, modified lognormal fit to the data sets.

Figure 3 contains several typical ASD samples for three different soil types. Since insufficient sieve cut data is available to describe the lower portion (< 0.42 mm) of these distributions, only a three-parameter, modified lognormal form was used to represent the distributions. The curve-fit parameters are presented in table 2 for these ASDs. One of the ASDs, the Reading soil, is the same one shown in figure 1, which represents a distribution with a very high percentage of large aggregates. The silt loam Ulysses soil (fine-silty, mixed, mesic, Aridic Haplustoll) contains the highest percentage of erodible aggregates (< 0.42 mm) and fewer large aggregates than either of the other two distributions. However, this soil sample still exhibits a sharp rise in the upper tail that cannot be accurately represented by a standard lognormal distribution. The silt loam Keith soil (fine-silty, mixed, mesic, Aridic Argiustoll) has a distribution bracketed by the other two soil's ASDs.

Summary and Conclusions

Modified forms of the standard lognormal functions can be used effectively to describe a broader range of ASDs determined from sieving field samples. The modified methods assume that either a limiting, nonzero, minimum size and/or a finite maximum size exists, which is normally true for ASDs. Therefore, the modified lognormal forms usually can represent a size distribution more accurately, especially at the upper and lower tails, than a standard lognormal function when sufficient sieve cut data is available to describe the tails. A more accurate description of ASDs helps depict wind erosion processes in greater detail and allows models such as WEPS to better simulate them. A computer program was developed to aid in the quick determination of either the standard or modified lognormal parameters.

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