Statistical Failure Analysis with Application to the Design of Nuclear Components Fabricated From Silicon Carbide

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Outline

• Introduction

• Weibull Distribution

• Estimating Parameters from Failure Data

• Bias & Confidence Bounds – Parameter Estimates

• Size Effects and System Reliability

• Confidence Bounds on Component Reliability

Throughout the presentation concepts will be clarified using a component represented by half of a spherical shell with a load concentrated on a small circular area, i.e., the SiC test component reported on in ORNL/TM-2008/167.
Characterizing Tensile Strength as a Random Variable

Ceramics exhibit low fracture toughness ($K_{IC}$) with a corresponding low strain tolerance.

High strength and low fracture toughness both lead to critical crack lengths that are beyond the resolution of current NDE equipment.

This leads to a distribution of undetectable “critical flaws” (fracture mechanics definition) in ceramics. Whether a flaw is a critical defect depends on its length and orientation to applied loads.

Thus actual defect distributions account for flaw size and flaw orientation relative to applied loads. This defect distribution tends to present as large variations in observed fracture strength.

In addition, the distribution of defects leads to an apparent decrease in tensile strength as the size of the component increases. This is the so-called strength-size effect, i.e., with bigger components there is an increased chance that larger more deleterious flaws are present.

In summary, tensile strength must be treated as a random variable.
Treating strength as a random variable demands that the engineer must tolerate a finite risk of unacceptable performance. This risk of unacceptable performance is quantified by a component's probability of failure. The primary concern of the engineer is minimizing this risk of failure in a safe and economical manner.

“Choosing” a distribution can be somewhat of a qualitative and subjective process. We stress that the physics that underlie a problem should indicate an appropriate choice. However, most times the engineer is left with somehow establishing a rational choice, and too often histograms and their shapes are relied on.

An attempt should be made to match the mathematics with the physics of the problem (appealing to extreme value distributions to represent load and strength). In addition, there are quantitative tools that can aid the engineer in his/her selection. These tools are known as goodness-of-fit tests, e.g.,

• Anderson-Darling Goodness-of-Fit Test

Usually these types of tests will only indicate when the engineer chooses badly. For ceramics, the industry has focused on the two parameter Weibull distribution. This is a Type III minimum extreme value statistic. Thus physics and mathematics drive this selection.
Two Parameter Weibull Distribution

The ceramics and glass industry have universally adopted the Weibull distribution. The Weibull distribution is an extreme value distribution and this makes the distribution an appropriate choice in representing the underlying probability distribution function for tensile strength. We are looking to predict the minimum value of tensile strength.

A two-parameter formulation and a three-parameter formulation are available for the Weibull distribution. However, the two-parameter formulation usually leads to a more conservative estimate for the component probability of failure. The two-parameter Weibull probability density function is given by the expression

\[
f(\sigma) = \left( \frac{\alpha}{\beta} \right) \left( \frac{\sigma}{\beta} \right)^{\alpha-1} \exp \left[ -\left( \frac{\sigma}{\beta} \right)^{\alpha} \right]
\]

for \( \sigma > 0 \), and

\[
f(\sigma) = 0
\]

for \( \sigma \leq 0 \).
The cumulative distribution is given by the expression

\[ F(\sigma) = 1 - \exp\left(-\left(\frac{\sigma}{\beta}\right)^\alpha\right) \]

for \( \sigma > 0 \), and

\[ F(\sigma) = 0 \]

for \( \sigma \leq 0 \). Here \( \alpha \) (a scatter parameter) and \( \beta \) (a central location parameter) are distribution parameters that are typically referred to as the Weibull modulus and the Weibull scale parameter, respectively.

In the ceramics literature when the two-parameter Weibull formulation is adopted then "\( m \)" is used for the Weibull modulus \( \alpha \), and \( \sigma_0 \) is used to represent \( \beta \).

There is a tendency to overuse the "\( \sigma \)" symbol (e.g., \( \sigma_\theta \), \( \sigma_\phi \), \( \sigma_i \)-failure observation, and \( \sigma_i \)-threshold stress, etc.). Throughout this presentation the use of the symbol "\( \sigma \)" should be apparent to the reader given the context in which it appears.
Parameter Estimation Theory - Preliminaries

The parameters associated with a distribution must be estimated on the basis of samples obtained from the population the distribution is modeling. The role of sampling as it relates to the statistical inference and parameter estimation is outlined in the figure in the next overhead.

The point is to construct a mathematical model that captures the population under study. This requires

• inferring the type of distribution that best characterizes the population; and

• estimating parameters once the distribution has been established.

Thus sampling a population will yield information in order to establish values of the parameters associated with the chosen distribution.
Assuming tensile strength is represented by the random variable $X$

### Experimental Observations - MOR bars or Tensile Specimens

\[ \{ x_1, x_2, \ldots, x_n \} \]

Construct histogram to simulate $f_X(x)$

### Familiar Statistics

- \[ \bar{x} = \frac{\sum x_i}{n} \]
- \[ s^2 = \frac{\sum (x_i - \bar{x})^2}{n - 1} \]

### Realizations of random variable $X$:

\[ 0 < x < +\infty \]

Assume random variable is characterized by the distribution $f_X(x)$

### Inferences on $f_X(x)$
Once the type of distribution has been made, the next step involves parameter estimation. There are two types of parameter estimation

- Point Estimates
- Interval Estimates

**Point estimation** is concerned with the calculation of a single number, from a sample of observations, that “best” represents the parameters associated with a chosen distribution.

**Interval estimation** goes further and establishes a statement on the confidence in the estimated quantity. The result is the determination of an interval indicating the range wherein the true population parameter is located. This range is associated with a level of confidence.

For a given number of samples, increasing the interval range increases the level of confidence. Alternatively, increasing the sample size will tend to decrease the interval range for a given level of confidence.

The best possible combination is a large confidence and small interval size.
The endpoints of the interval range define what is known as “confidence bounds.”
Bias and Invariance

In general, the objective of parameter estimation is the derivation of functions, i.e., estimators, that are dependent on failure data, and that yield in some sense optimum estimates of the underlying population parameters.

Various performance criteria can be applied to ensure that optimized estimates are obtained consistently. Two important criteria are:

- **Estimate Bias**
- **Estimate Invariance**

Bias is a measure of the deviation of the estimated parameter value from the expected value of the population parameter. The values of point estimates computed from a number of samples will vary from sample to sample. In this context, the word sample specifically implies a group of failure strengths.

If enough samples are taken one can generate statistical distributions for the point estimates, as a function of sample size. If the mean of a distribution representing the parameter estimate is equal to the expected value of the parameter, the associated estimator is said to be unbiased.
There are three typical methods utilized in obtaining point estimates of distribution functions:

- **Method of moments (not discussed)**
- **Linear regression techniques (very briefly discussed)**
- **Likelihood techniques (estimation approach of choice)**

If an estimator yields biased results, the value of an individual estimate can easily be corrected if the estimator is invariant. An estimator is invariant if the bias associated with the estimated parameter value is not functionally dependent on the true distribution parameters that characterize the underlying population.

An example of an estimator that is not invariant is the linear regression estimators for the three-parameter Weibull distribution.

The maximum likelihood estimator (MLE) for a two-parameter Weibull distribution is invariant.
Ranking Schemes – Probability of Failure

Consider an experiment where the tensile strength data has been collected. The tensile strength data is identified as the dependent variable since the individual conducting the test can not control the value of this parameter – the material does. We need to adopt an independent random variable. Consider the ranked probability of failure associated with each tensile strength value depicted in the generic table below.

<table>
<thead>
<tr>
<th>Experimental Data</th>
<th>Probability of Failure $P_i (= x_i)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Strength ($y_i$)</td>
<td></td>
</tr>
<tr>
<td>$y_1$</td>
<td>$x_1$</td>
</tr>
<tr>
<td>$y_2$</td>
<td>$x_2$</td>
</tr>
<tr>
<td>$y_3$</td>
<td>$x_3$</td>
</tr>
<tr>
<td>…</td>
<td>…</td>
</tr>
<tr>
<td>$y_n$</td>
<td>$x_n$</td>
</tr>
</tbody>
</table>

For linear regression estimators the choice of ranking scheme impacts the values of the parameter estimates. For maximum likelihood estimators ranking schemes are simply used to plot data and the effects are cosmetic.

Note: Although the table to the left shows $y$ dependent on $x$, in typical Weibull plots $P_i$ is the vertical axis and strength is the horizontal axis. This causes confusion, especially using commercial spread sheet software to estimate parameters via linear regression.
Ordered statistics are employed to rank failure data. A number of ranking schemes for $P_i$ have been proposed in the literature. One type of ranking scheme is given by the expression

\[
F(x_i) = P_i = \frac{i - 0.3}{n + 0.4}
\]

Another ranking scheme proposed by Nelson (1982) had found wide acceptance. Here

\[
F(x_i) = P_i = \frac{i - 0.5}{n}
\]

This estimator yields less bias than the median rank estimator, or the mean rank estimator. It is also the estimator accepted for use in ASTM C1239, and ISO Designation FDIS 20501.

Minimizing bias drives many decisions in parameter estimation.
The B&W-93060 material (Data Set #9) from ORNL/TM-2008/167 is used to illustrate the slight graphical differences in the probability of failure estimators.
Method of Maximum Likelihood

The method of maximum likelihood is the most commonly used estimation technique for brittle material strength because the estimators derived by this approach maintain some very attractive features.

Let \((X_1, X_2, X_3, \ldots, X_n)\) be a random sample of size \(n\) drawn from an arbitrary probability density function with one distribution parameter, i.e.,

\[ f_X(x, \theta) \]

Here \(\theta\) is an unknown distribution parameter. The likelihood function of this random sample is defined as the joint density of the \(n\) random variables

\[
L = \text{Likelihood Function} \\
= \prod_{i=1}^{n} f_X(x_i, \theta) \\
= f_X(x_1, \theta) f_X(x_2, \theta) \cdots f_X(x_n, \theta)
\]
Often times it is much easier to manipulate the logarithm of the likelihood function, i.e.,

\[ \mathcal{L} = \ln \left\{ \prod_{i=1}^{n} f_{X}(x_i, \theta_1, \theta_2, \ldots, \theta_k) \right\} \]

Here \( k \) represents the number of parameters associated with a particular distribution. The maximum likelihood estimator (MLE) of \( \theta \) identified as \( \hat{\theta} \), is the root of the expression obtained by equating the derivative of \( \mathcal{L} \) to zero

\[ \frac{\partial \mathcal{L}}{\partial \theta} = 0 \]

If there is more than one parameter associated with a distribution, then derivatives of the log likelihood function are taken with respect to each unknown parameter, and each derivative is set equal to zero, i.e.,

\[ \frac{\partial \mathcal{L}}{\partial \theta_1} = 0 \quad , \quad \frac{\partial \mathcal{L}}{\partial \theta_2} = 0 \quad , \quad \ldots \quad , \quad \frac{\partial \mathcal{L}}{\partial \theta_k} = 0 \]

When more than one parameter must be estimated often times the system of equations obtained by taking the derivative of the log likelihood function must be solved in an iterative fashion, e.g., as is done with the two parameter Weibull distribution.
The next two graphs illustrate how a first guess, and then a subsequent iteration affects the likelihood function. When

\[ f(x, \theta_1, \theta_2) = f(\sigma, m, \sigma_\theta) = \left( \frac{m}{\sigma_\theta} \right) \left( \frac{\sigma}{\sigma_\theta} \right)^{m-1} \exp \left[ -\left( \frac{\sigma}{\sigma_\theta} \right)^m \right] \]

then the first graph below plots this probability density function based on the first guess of \( m (= \theta_1) \) and \( \sigma_\theta (= \theta_2) \). All nine test values fall to the right of the peak for this iteration on the parameter values. If the sampling was truly random the test values should be more evenly spaced.
The next graph represents an iteration on the estimated distribution parameter values. Note the vertical scale has been maintained from the previous graph.

The shape and position of the probability density function appear to be a much better fit to the nine data points. Again, we base judgment on the assumption that our data values represent a random sample and they should therefore span the range. Note for small sample sizes this assumption can easily break down.
In both figures nine arrows point to the associated values of the joint probability density function for each of the nine failure strengths. The product of these nine values represents the value of the likelihood function for each choice of distribution parameters.

A simple inspection is sufficient to conclude that the likelihood from the latter iteration is greater than the likelihood from the former. If the latter choice of parameters is considered more acceptable, then this would indicate that obtaining a “best” set of distribution parameters involves maximizing the likelihood function.

Two important properties of maximum likelihood estimators

1. Maximum likelihood estimators yield unique solutions

2. Estimates rapidly converge to the true parameters as the sample size increases
MLE – Two Parameter Weibull Distribution

Let \( \sigma_1, \sigma_2, \ldots, \sigma_N \) represent realizations of the ultimate tensile strength (a random variable) in a given sample, where it is assumed that the ultimate tensile strength is characterized by the two-parameter Weibull distribution. As noted in the previous section the likelihood function associated with this sample is the joint probability density evaluated at each of the \( N \) sample values. Thus this function is dependent on the two unknown Weibull distribution parameters \((m, \sigma_\theta)\). The likelihood function for an uncensored sample under these assumptions is given by the expression

\[
L = \prod_{i=1}^{N} \left( \frac{\hat{m}}{\hat{\sigma}_\theta} \right) \left( \frac{\sigma_i}{\hat{\sigma}_\theta} \right)^{\hat{m} - 1} \exp \left[ - \left( \frac{\sigma_i}{\hat{\sigma}_\theta} \right)^{\hat{m}} \right]
\]

Here \( \hat{m} = \theta_1 \) and \( \hat{\sigma}_\theta = \theta_2 \) designate estimates of the true distribution parameters \( m \) and \( \sigma_\theta \).
A system of equations obtained by differentiating the log likelihood function and setting the derivatives equal to zero for a uncensored sample is given by

\[ \sum_{i=1}^{N} \left( \sigma_i \right)^{\hat{m}} \ln \left( \sigma_i \right) - \frac{1}{N} \sum_{i=1}^{N} \ln \left( \sigma_i \right) - \frac{1}{\hat{m}} = 0 \]

And

\[ \hat{\sigma}_\theta = \left[ \left( \sum_{i=1}^{N} \left( \sigma_i \right)^{\hat{m}} \right) \frac{1}{N} \right]^{1/\hat{m}} \]

The top equation is solved first for \( \hat{m} \). Subsequently \( \hat{\sigma}_\theta \) is computed from the second expression. Obtaining a closed form solution for the first equation is not possible. This expression must be solved numerically. WeibPar solves these equations in an iterative fashion.
Using the maximum likelihood estimators from the previous slide on Data Set #9 from ORNL/TM-2008/167 yields the following estimates for the Weibull parameters. A graph of the data and the Weibull CDF is also provided.

<table>
<thead>
<tr>
<th>Estimation Method</th>
<th>Rank Formula</th>
<th>Weibull Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>MLE</td>
<td>(i - 0.5) / N</td>
<td>m = 5.68, σ₀ = 927.2</td>
</tr>
</tbody>
</table>
Multiple Flaw Distributions (C.A. Johnson)

The previous discussion assumes that single distribution of flaws is present throughout the specimens being tested. Real ceramic materials may contain two or more types of defects, each with its own characteristic flaw size distribution. This can be easily verified using careful fractographic techniques.

The other indication of multiple flaw distributions is a distinctive “knee” in the data. This is depicted in the figure to the right. This figure appears in ASTM C 1239.
The knee in the curve can appear as it does in the previous graph, or the curvature can be reversed as shown to the right. This figure appears in a GE report (1979) by C.A. Johnson.

One can use the manner in which a knee is generated, i.e., how the data deviates from linearity to deduce information concerning the nature of the flaw distributions present.

Consider a group of test specimens that when failed, have two distinctly different types of fracture origins. Some specimens fail from flaw type “A” while the remainder fail from flaw type “B.”
There are at least three ways in which these two flaw populations are present in the test specimens, i.e., the sample.

- Both flaw distributions are present in every test specimen. This is known as “Concurrent Flaw Populations.”

- Within a group of specimens any given specimen may contain flaws from distribution A, or from distribution B, but not from both. This is known as “Mutually Exclusive Flaw Populations.”

- Within a group of specimens, flaw distribution A may be present in all specimens, while distribution B may be present in only some test specimens. This is known as “Partially Concurrent Flaw Populations.”

A larger number of cases must be considered than the three above if more than two flaw distributions are active.
Examples of the three types of flaw distributions are as follows.

*Concurrent Flaw Distributions* – A group of test specimens machined from a ceramic billet which contains defects distributed throughout the volume. Each specimen then contains both machining flaws on the surface and volume defects interior to the test specimen.

*Exclusive Flaw Distributions* – A group of test specimens comprised of two subgroups purchased from two different manufacturers.

*Partially Concurrent Distributions* - A group of pressed and sintered test specimens which were all sintered in the same furnace, but could not be sintered in a single furnace cycle. The specimens sintered at the longer cycle would contain elongated grains (considered a deleterious flaws) and all the specimens would have strength degrading inclusions present from the powder preparation.

The parameter estimation methods presented here assumes that if *multiple flaw populations are present, then they are concurrent flaw distributions*. As indicated above, partially concurrent distributions point to processing methods that have not, or are not mature. In addition, it is quite typical for a manufacturer of ceramic components to identify one material supplier, and this would minimize the presence of exclusive flaw distributions.
MLEs for Multiple Flaw Distributions

The likelihood function for the two-parameter Weibull distribution where concurrent flaw distributions are present (known as a censored sample) is defined by the expression

\[
L = \left\{ \prod_{i=1}^{r} \left( \frac{\hat{m}}{\hat{\sigma}_i} \right) \left( \frac{\sigma_i}{\hat{\sigma}} \right)^{\hat{m} - 1} \exp \left[ - \left( \frac{\sigma_i}{\hat{\sigma}} \right)^{\hat{m}} \right] \right\} \prod_{j=r+1}^{N} \exp \left[ - \left( \frac{\sigma_j}{\hat{\sigma}} \right)^{\hat{m}} \right]
\]

This expression is applied to a sample where two or more active concurrent flaw distributions have been identified from fractographic inspection. For the purpose of the discussion here, the different distributions will be identified as flaw types A, B, C, etc. When the expression above is used to estimate the parameters associated with the A flaw distribution, then \(r\) is the number of specimens where type-A flaws were found at the fracture origin, and \(i\) is the associated index in the first summation. The second summation is carried out for all other specimens not failing from type-A flaws (i.e., type-B flaws, type-C flaws, etc.). Therefore the sum is carried out from \((j = r + 1)\) to \(N\) (the total number of specimens) where \(j\) is the index in the second summation. Accordingly, \(\sigma_i\) and \(\sigma_j\) are the maximum stress in the \(i^{th}\) and \(j^{th}\) test specimens at failure, respectively.
The system of equations obtained by differentiating the log likelihood function for a censored sample is given by

\[
\sum_{i=1}^{N} \left( \frac{\hat{\sigma}_i}{\hat{m}} \right)^{\hat{m}} \ln \left( \frac{\sigma_i}{\hat{\sigma}_i} \right) = - \frac{1}{r} \sum_{i=1}^{r} \ln \left( \frac{\sigma_i}{\hat{\sigma}_i} \right) - \frac{1}{\hat{m}} = 0
\]

and

\[
\hat{\sigma}_\theta = \left[ \left( \sum_{i=1}^{N} \left( \frac{\hat{\sigma}_i}{\hat{m}} \right) \right) \frac{1}{r} \right]^{-1/\hat{m}}
\]

where:

\( r \) = the number of failed specimens from a particular group of a censored sample.
Size Effects – Test Specimens

The failure behavior in ceramic materials is sudden and catastrophic. This behavior fits the description of failure in a series system, a weakest-link system. The probability of failure of a discrete element at a point (a link) in the component can easily be related to the overall probability of failure of the component (the chain).

Finite element software is used to describe the state of stress throughout the component. Thus a component is discretized, and the reliability of each discrete element must be related to the overall reliability of the component. The reliability of a continuum element is defined as

\[ R_i = \exp \left( - \left( \frac{\sigma_i}{\sigma_0} \right)^m \Delta V_i \right) \]

The volume of an arbitrary continuum element is identified by \( \Delta V \). In this expression \( \sigma_0 \) is the Weibull material scale parameter and can be described as the Weibull characteristic strength of a specimen with unit volume loaded in uniform uniaxial tension. This is a material specific parameter that is utilized in the component reliability analyses that follow. The dimensions of this parameter are stress \( \cdot (\text{volume})^{1/m} \).
The requisite size scaling is introduced by the previous equation. To demonstrate this, take the natural logarithm of this expression twice, i.e.,

\[
\ln \left[ \ln \left( \mathcal{R}_i \right) \right] = \ln \left( -\left( \frac{\sigma}{\sigma_0} \right)^m \Delta V \right)
\]

Manipulation of this expression yields

\[
\ln(\sigma) = -\left( \frac{1}{m} \right) \ln(\Delta V) + \left( \frac{1}{m} \right) \ln \ln \left( \frac{1}{\mathcal{R}_i} \right) + \ln(\sigma_0)
\]

With

\[
y = \ln(\sigma)
\]
\[
x = \ln(\Delta V)
\]
\[
m_1 = -\frac{1}{m}
\]

\[
b = \frac{1}{m} \ln \ln \left( \frac{1}{\mathcal{R}_i} \right) + \ln(\sigma_0)
\]
then it is apparent that the double log equation has the form of a straight line, i.e.,
\[ y = m_f x + b, \]
and plots as follows.

Consider several groups of test specimens fabricated from the same material. The specimens in each group are identical with each other, but each group has a different gage section such that \( \Delta V \) (which is now identified as the gage section volume; or \( \Delta A \) which is identified as the gage area) is different from one group to the next. Estimate Weibull parameters \( m \) and \( \sigma_0 \) from the pooled failure data obtained from each group (pooling techniques are not a part of this discussion).
After the Weibull parameters are estimated, the line for \( y = m_i x + b \) can be plotted that corresponds to say \( R_i = 50\% \) (i.e., the 50\(^{th}\) percentile). This value should correlate well with the median values in each group, if the number in each group is large.

Plot this specific curve as a function of the gage volumes (\( \Delta V \)) or gage area (\( \Delta A \)) for each group, as in the figure to the right. If no size effect is present, then median failure strengths of the groups will fall close to a horizontal line. This would indicate no correlation between gage geometry and the median strength value. A systematic variation away from a horizontal line indicates that a size effect is present. The figure to the right appears in Johnson and Tucker (1991) supports the existence of a “Weibull” size effect in the SiC material tested.
We can also view this phenomenon in a classical Weibull probability graph. Here data sets representing tensile specimen geometries for three different gage volumes are depicted.

The data sets have been generated through the use of Monte Carlo simulation techniques.

<table>
<thead>
<tr>
<th>m</th>
<th>Sig Not</th>
</tr>
</thead>
<tbody>
<tr>
<td>45</td>
<td>47000</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Tensile Volume</th>
<th>Monte-Carlo</th>
<th>Actual</th>
</tr>
</thead>
<tbody>
<tr>
<td>V</td>
<td>Sig Theta</td>
<td>Sig Theta</td>
</tr>
<tr>
<td>1</td>
<td>47,000</td>
<td>46,903</td>
</tr>
<tr>
<td>4</td>
<td>45,574</td>
<td>45,322</td>
</tr>
<tr>
<td>16</td>
<td>44,192</td>
<td>43,974</td>
</tr>
</tbody>
</table>

The preceding discussion took place relative to test specimens with uniaxial stress states. The next step is to extend these concepts and capture the effects of multiaxial stress states present in components.
Parameter Estimation – Bias

A certain amount of intrinsic variability occurs due to sampling error. This error is associated with the fact that only a limited number of observations are taken from an infinite (assumed) population.

Bias - Deviation of the expected value of the estimated parameter from the true parameter. This is the tendency of a particular estimator to give consistently high or consistently low estimates relative to the true value.

Once it is recognized that the estimates of the Weibull modulus and characteristic strength will vary from sample to sample, these estimates can be treated as random variables (i.e., statistics).

For a population characterized by a two parameter Weibull distribution the expected value of the distribution parameters should approach the true distribution parameters in the limit as the number of samples tested increases.

\[
E[\hat{m}] = \int_{-\infty}^{+\infty} \hat{m} f_{\hat{m}}(\hat{m}) d\hat{m} \\
\Rightarrow \frac{1}{k} \sum_{j=1}^{k} \hat{m}_j \\
\cong m \text{ (true Weibull modulus)}
\]

\[
E[\hat{\sigma}_\theta] = \int_{-\infty}^{+\infty} \hat{\sigma}_\theta f_{\hat{\sigma}_\theta}(\hat{\sigma}_\theta) d\hat{\sigma}_\theta \\
\Rightarrow \frac{1}{k} \sum_{j=1}^{k} (\hat{\sigma}_\theta)_j
\]
Trends in bias associated with an estimator can be monitored using Monte Carlo simulation to ascertain trends. With

$$\rho_{\hat{m}} = \frac{E(\hat{m}_i)}{m}$$

then this ratio is represented by the dashed curve which is an average value for $\rho_{\hat{m}}$ given the simulation size. If the estimator for the Weibull modulus (an MLE was used in this example) was unbiased, then

$$\rho_{\hat{m}} = 1$$

We see that this is only true in the limit as the number of specimens increases.

The ability to quantify bias allows us to remove it using the value $\rho_{\hat{m}}$, as long as the estimator used is invariant, i.e., if the Monte Carlo simulation outlined above works for any set of true distribution parameters chosen in Step #1. This is not always possible for all the estimators available.
If one uses maximum likelihood estimators to compute the Weibull characteristic strength, then the estimate of the parameter is essentially unbiased.

This can be seen in the graph to the right where the dashed line is essentially equal to one for nearly all values of the number of specimens per sample.
Confidence Bounds

Confidence bounds quantify the uncertainty associated with a point estimate of a population parameter.

The values used to construct confidence bounds are based on percentile distributions obtained from Monte Carlo simulations discussed in the previous overheads. For example, given a fixed sample size \((n)\) and a simulation that contains 10,000 estimates, then after ranking the estimates in numerical order

\[
\begin{align*}
1,000\text{th Estimate} & - 10\text{th Percentile} \\
2,000\text{th Estimate} & - 20\text{th Percentile} \\
9,000\text{th Estimate} & - 90\text{th Percentile}
\end{align*}
\]

The 10th and 90th percentile define a range of values where the user is 80% confident that the true value of the parameter estimate lies between these two values. Confidence bounds are closely associated with the concept of hypothesis testing.

The theorems derived by Thoman, Bain & Antle (1969) allows one to easily compute confidence bounds on MLE parameter estimates for a two parameter Weibull distribution. The approach to compute these bounds on each parameter estimate is available in ASTM C1239 and WeibPar.
Effective Area – Spherical Fuel Particle

With

\[ P_f = 1 - \exp \left[ -\left( \frac{\sigma_{\text{max}}}{\sigma_\theta} \right)^m \right] \]

where

\[ \sigma_{\text{max}} = \text{maximum uniaxial tensile stress in a test specimen at failure} \]
\[ \sigma_\theta = \text{the Weibull characteristic strength} \]

then if fractography indicates that the failure originates from the inner surface of the particle under the load, then the expression above can also be expressed as

\[ P_f = 1 - \exp \left[ -\int_{A} \left( \frac{\sigma}{(\sigma_\theta)_A} \right)^{m_A} dA \right] \]

Closed form expressions for the effective volume \( (A_{\text{eff}}) \) of standard test specimens can be obtained by equating these two expressions in a manner outlined in ASTM C 1683.
For test specimen geometries not found in the ASTM standard, specifically the test specimen geometry identified in ORNL/TM-2008/167 for the spherical fuel particle, a numerical approach can be used to derive values for an effective gage area, $A_{\text{eff}}$ (and a similar expression for $V_{\text{eff}}$) can be derived in the following manner. Identify the estimated Weibull modulus as

$$\tilde{m}_A = m_A$$

Also identify

$$\sigma^* = \left(\sigma_0\right)_A$$

as a parameter. Now

$$P_f = 1 - \exp\left[-\int_A \left(\frac{\sigma}{\sigma^*}\right)^{\tilde{m}_A} dA\right]$$

and rearranging yields

$$P_f = 1 - \exp\left[-\left(\frac{\sigma_{\text{max}}}{\sigma^*}\right) \int_A \left(\frac{\sigma}{\sigma_{\text{max}}}\right)^{\tilde{m}_A} dA\right]$$
Identify

\[ A_{\text{eff}} = \int_V \left( \frac{\sigma}{\sigma_{\text{max}}} \right)^{\tilde{m}_A} dA \]

Now

\[ P_f = 1 - \exp \left[ A_{\text{eff}} \left( \frac{\sigma_{\text{max}}}{\sigma^*} \right)^{\tilde{m}_A} \right] \]

Solving this last equation for the effective area where as noted above \( \sigma^* \) is treated as a parameter yields

\[ A_{\text{eff}} = \frac{-\ln \left( 1 - P_f \right)}{\left( \frac{\sigma_{\text{max}}}{\sigma^*} \right)^{\tilde{m}_A}} \]
At this point a numerical approach is employed whereby finite element analysis is utilized along with Weibull analysis to evaluate the effective volume. The four step numerical approach is as follows:

1. Conduct a finite element analysis to obtain the stress field throughout the test specimen. This analysis will also provide $\sigma_{max}$.

2. Estimate $m_A$ from failure data.

3. Numerically evaluate

$$P_f = 1 - \exp \left[ -\int_A \left( \frac{\sigma}{\sigma^*} \right)^{m_A} dA \right]$$

using CARES. Note that $m_A$ from Step #2 is used with an arbitrarily selected value of $\sigma^*$.

4. With $\sigma^*$, $P_f$ and $\sigma_{max}$ solve for $A_{eff}$

This four step approach is similarly utilized to compute $V_{eff}$. The technique for obtaining effective areas and volumes is available in CARES and WeibPar.
The effective area \((A_{\text{eff}})\) is a constant for a given specimen geometry. One can deduce that an increase in the applied load will increase both \(P_f\) as well as \(\sigma_{\text{max}}\). Both values compensate each other in the expression

\[
A_{\text{eff}} = \frac{-\ln\left(1 - P_f\right)}{\left(\frac{\sigma_{\text{max}}}{\sigma^*}\right)^{\tilde{m}_A}}
\]

keeping the effective area a constant when the magnitude of the load is varied. In addition, the parameter \(\sigma^*\) will affect the value of \(P_f\) obtained from Step #3 where

\[
P_f = 1 - \exp\left[-\int_A \left(\frac{\sigma}{\sigma^*}\right)^{\tilde{m}_A} dA\right]
\]

However, in the first equation changes in \(P_f\) will be compensated by changes in \(\sigma^*\) such that \(A_{\text{eff}}\) once again is unaffected. The only parameter that has an effect on the value of \(A_{\text{eff}}\) is the Weibull modulus. Once an estimate for the Weibull modulus is obtained the value of the modulus remains unchanged in the analysis above.
Consider the geometry of the half sphere test specimens outlined in ORNL/TM-2008/167. A generic 2D axisymmetric model of the test specimen is given to the right. For this test specimen:

• a pressure is applied to a circular contact area

• the maximum tensile stress occurs on inner surface directly below the center of the load

• *WeibPar* and *CARES* were used to calculate the effective area (on the inner surface) and the Weibull material scale parameter, \( \sigma_0 \); *WeibPar* utilizes information obtained from the finite element analysis to make these calculations.
The mesh is optimized using a convergence criterion based on the computed effective area.

The mesh contains 4,400 elements. Very thin elements are along the inner and outer surfaces.
MLE2B Weibull modulus
Characteristic strength
Effective area
Computed material scale parameter

\[ m_A = 5.675 \]
\[ \sigma_\theta = 927.2 \text{ MPa} \]
\[ A_{\text{eff}} = 0.0110 \text{ mm}^2 \]
\[ \sigma_0 = 418.9 \text{ MPa} \cdot \text{mm}^{2/5.675} \]
Component Reliability – Series System

The ability to account for size effects of an individual element was introduced through the expression appearing earlier, i.e.,

\[ R_i = \exp\left( -\left( \frac{\sigma_i}{\sigma_0} \right)^{m_y} \Delta V_i \right) \]

Now a general expression for the probability of failure for a component is derived. Under the assumptions that the component consists of an infinite number of elements (i.e., the continuum assumption) and that the component is best represented by a series system, then

\[ P_f = 1 - \lim_{k \to \infty} \left( \prod_{i=1}^{k} R_i \right) \]
substitution leads to

\[ P_f = 1 - \exp \left( -\lim_{k \to \infty} \sum_{i=1}^{k} \left( \frac{\sigma}{\sigma_0} \right)^{m_V} \Delta V_i \right) \]

The limit inside the bracket is a Riemann sum. Thus

\[ P_f = 1 - \exp \left[ -\int \left( \frac{\sigma}{(\sigma_0)_V} \right)^{m_V} dV \right] \]

Weibull (1939) first proposed this integral representation for the probability of failure. The expression is integrated over all tensile regions of the specimen volume if the strength-controlling flaws are randomly distributed through the volume of the material, or over all tensile regions of the specimen area if flaws are restricted to the specimen surface. For failures due to surface defects the probability of failure is given by the expression

\[ P_f = 1 - \exp \left[ -\int \left( \frac{\sigma}{(\sigma_0)_A} \right)^{m_A} dA \right] \]
**Multiaxial Reliability Models**

Over the years a number of reliability models have been presented that extend the uniaxial integral formats given on the previous slide to multiaxial states of stress.

A number of reliability models have been presented in the literature that assess component reliability based on multiaxial states of stress. The two monolithic models highlighted here include the principle of independent action (PIA) model and Batdorf’s model.

The PIA model is presented in the next section. This is a phenomenological model.

Batdorf’s model brings all the rigor of fracture mechanics to a probability of failure analysis including the ability to make predictions based on flaw types.

For either model the component probability of failure is expressed in the following generic formats

\[
(P_f)_V = 1 - \exp\left[-\int \psi \, dV \right] \quad \text{or} \quad (P_f)_A = 1 - \exp\left[-\int \psi \, dA \right]
\]

where \( \psi \) is identified as a failure function per unit volume or area. What remains is the specification of the failure function \( \psi \) for each reliability model.
For the principle of independent action (PIA) model:

\[ \psi = \left( \frac{\sigma_1}{\sigma_0} \right)^m + \left( \frac{\sigma_2}{\sigma_0} \right)^m + \left( \frac{\sigma_3}{\sigma_0} \right)^m \]

where \( \sigma_1, \sigma_2 \) and \( \sigma_3 \) are the three principal stresses at a given point. Recall that \( \sigma_0 \) is the Weibull material scale parameter and can be described as the Weibull characteristic strength of a specimen with unit volume, or area, loaded in uniform uniaxial tension.

The PIA model is the probabilistic equivalent to the deterministic maximum stress failure theory. The PIA model has been widely applied in brittle material design. However, the PIA model does not specify the nature of the defect causing failure. The fact that the model is phenomenological does not imply that the model is not useful. The simplicity of phenomenological models can often times be a strength, not a weakness.

Details of the Batdorf model are not presented here due to time constraints.
Bootstrap Bounds on Component Reliability Calculations

Bootstrap methods characterize uncertainty in estimates that arise from random sampling error, i.e., errors due to testing a finite number of test specimens that represent an assumed infinite sample population. As the term bootstrap implies, this method literally "pulls itself up by its bootstraps." The methodology is a re-sampling technique. The original data set used to estimate Weibull parameters is re-sampled using numerical simulation and reevaluated – many times over. Each simulated data set is generated such that the number of sample points matches the original finite number of test specimens.

The parametric bootstrap technique is presented. In parametric bootstrapping an assumed distribution is utilized. Here the assumed distribution is the two parameter Weibull distribution. In addition, maximum likelihood estimators are employed to estimate parameters.

Bootstrap methods are capable of characterizing confidence bounds as well as bias associated with estimates of the Weibull parameters. When combined with the information provided by the component effective volume or effective area, the method is capable of characterizing confidence bounds as well as bias associated with estimates of component probability of failure. We focus on component reliability by demonstrating the step-by-step methodology implemented within WeibPar and CARES.
Based on the test values for Data Set #9 in ORNL/TM-2008/167 the effective areas for the test specimen and the pressurized sphere are given beneath each finite element stress plot.

**Test Specimen**

\[ T S(A_{eff}) = 0.01101 \text{ mm}^2 \text{ (original)} \]

Previously the effective area of the test specimen was computed for the computed Weibull parameters from each simulation. A similar calculation is made for the pressurized sphere.

**Pressurized Sphere**

\[ comp(A_{eff}) = 0.6253 \text{ mm}^2 \text{ (original)} \]

20 MPa
We wish to establish bounds on the probability of failure for a thin wall sphere subject to an internal pressure. The half sphere with an applied central pressure load is our test specimen.

A sufficient amount of failure data must be available to compute high quality estimates for the Weibull distribution parameters. The question is how much data is “sufficient”? It is assumed that all failures take place along the inner surface under the center of the pressure load.

a) We begin to answer the question regarding sufficiency by estimating the Weibull parameters from the failure data. As before the Weibull modulus is

\[ \tilde{m}_A = 5.675 \]

and the Weibull characteristic strength is

\[ (\tilde{\sigma}_\theta)_A = 927.2 \text{ MPa} \]
b) Next, we begin the resampling process. A random number between 0 and 1 is generated. Take this value as $R_i$

c) Calculate a failure stress associated with the random number from (b) and the Weibull parameters from (a) using the expression

$$\sigma_i = \left( -\ln\left( \frac{R_i}{\bar{\sigma}_\theta} \right) \right)^{1/m_A}$$

d) Repeat steps (b) and (c) $N$ times, where $N$ is the original number of test specimen data values. For this particular data set $N = 31$.

**TABLE 1 – Simulated Data Set**

<table>
<thead>
<tr>
<th>$i$</th>
<th>$\sigma_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$Eq Above$</td>
</tr>
<tr>
<td>2</td>
<td>$Eq Above$</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>$N = 31$</td>
<td>$Eq Above$</td>
</tr>
</tbody>
</table>
e) Estimate Weibull parameters from the data set generated in the previous steps using maximum likelihood estimators (MLEs).

f) Repeat steps (b) through (e) as many times as is computational feasible carefully recording the simulated Weibull modulus and characteristic strength (see Table 2) are thus generated.

<table>
<thead>
<tr>
<th>(J)</th>
<th>(\bar{m}_A)</th>
<th>(\bar{\sigma}_\theta)</th>
<th>(A_{\text{eff}})</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>(\bar{m}_A)_1</td>
<td>(\bar{\sigma}_\theta)_1</td>
<td>(A_{\text{eff}})_1</td>
</tr>
<tr>
<td>2</td>
<td>(\bar{m}_A)_2</td>
<td>(\bar{\sigma}_\theta)_2</td>
<td>(A_{\text{eff}})_2</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>BS=2,000</td>
<td>(\bar{m}<em>A)</em>{BS}</td>
<td>(\bar{\sigma}<em>\theta)</em>{BS}</td>
<td>(A_{\text{eff}})_{BS}</td>
</tr>
</tbody>
</table>
We can extend the bootstrap process to generate bounds on the component (pressurized sphere) reliability for a pressurized sphere:

**g)** Establish the correspondence between the simulated Weibull moduli and the test specimen \((TS)\) effective area, i.e., \((m_{A})\) and \(TS(A_{eff})\). Also establish the correspondence between the simulated Weibull moduli and the effective area of the component (the pressurized sphere), i.e.,

\[
\begin{align*}
comp(A_{eff}) & = \frac{-\ln(1 - P_f)}{\left(\frac{\sigma_{max}}{\sigma^{*}}\right)} \\
& \left(\frac{J}{\left(A_{eff}\right)_{TS}}A\right)^{1/(m_{A})_{comp}}
\end{align*}
\]

**h)** Calculate the material material scale parameter in the sixth column of Table 3 (next slide) using the following expression:

\[
\begin{align*}
J\left(\sigma_{0}\right)_{A} &= J\left(\tilde{\sigma}_{\theta}\right)_{A} \left[TS\left(A_{eff}\right)_{J}\right]^{1/(m_{A})_{J}}
\end{align*}
\]

**i)** Calculate the component probability of failure in the seventh column of Table 3 using \(\sigma_{\text{max}}\) from the finite element analysis of the component and the following expression:

\[
\begin{align*}
comp\left(P_{f}\right)_{J} & = 1 - \exp \left\{-\left[comp\left(A_{eff}\right)_{J}\right]\left(\frac{\sigma_{max}}{J\left(\sigma_{0}\right)_{A}}\right)^{\left(m_{A}\right)_{J}}\right\}
\end{align*}
\]
j) As *WeibPar* stores and manipulates the data from Table 3, *CARES* performs the probability of failure calculations utilizing the finite element models.

k) Sort by $P_f$ in order to establish percentiles and then choose bounds based on the percentiles.

*WeibPar* calculates the confidence bounds on component reliability via integration with *CARES*. As *WeibPar* stores and manipulates the data from Table 2, *CARES* perform the probability of failure calculations on the finite element model.

**Table 3 - Bootstrap Component Reliability**

<table>
<thead>
<tr>
<th>J</th>
<th>$(\tilde{m}_A)_J$</th>
<th>$J(\bar{\sigma}_\theta)_A$</th>
<th>$TS(A_{eff})_J$</th>
<th>Comp $(A_{eff})_J$</th>
<th>$J(\sigma_0)_A$</th>
<th>Comp $(P_f)_J$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$(\tilde{m}_A)_1$</td>
<td>$1(\bar{\sigma}_\theta)_A$</td>
<td>$TS(A_{eff})_1$</td>
<td>Comp $(A_{eff})_1$</td>
<td>$1(\sigma_0)_A$</td>
<td>Comp $(P_f)_1$</td>
</tr>
<tr>
<td>2</td>
<td>$(\tilde{m}_A)_2$</td>
<td>$2(\bar{\sigma}_\theta)_A$</td>
<td>$TS(A_{eff})_2$</td>
<td>Comp $(A_{eff})_2$</td>
<td>$2(\sigma_0)_A$</td>
<td>Comp $(P_f)_2$</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
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<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>BS=2,000</td>
<td>$(\tilde{m}<em>A)</em>{BS}$</td>
<td>$BS(\bar{\sigma}_\theta)_A$</td>
<td>$TS(A_{eff})_{BS}$</td>
<td>Comp $(A_{eff})_{BS}$</td>
<td>$BS(\sigma_0)_A$</td>
<td>Comp $(P_f)_{BS}$</td>
</tr>
</tbody>
</table>
This figure depicts the bounds on component reliability for the data set used to generate the Weibull parameters. The blue diamond is the component probability of failure given the biased maximum likelihood Weibull parameters calculated. The extreme two data points (black diamonds) are the 5% and 95% confidence bounds. We are 90% certain that the actual component probability of failure falls between these two points. Also included are the Mean and Median probability of failure (green square and red triangle, respectively).
The question can be posed, what effect does the limited information (31 failure stresses in this case) have on the bounds on reliability? To answer this question the bootstrap technique can be rerun for a variety of specimen data set sizes. Please note that these are hypothetical results in the sense that if we really broke 9 more specimens to increase our specimen data set to 40 then it is unlikely that the recalculated Weibull parameters would be the same as for the original 31 data points.
Selected References


Presentation can be found at - http://academic.csuohio.edu/duffy_s/duffy.html