STATISTICAL ANALYSIS OF SINGLE PPTA FIBERS

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1 General Introduction

Single fiber tensile tests are often conducted to measure fiber properties of high strength polymer fibers, such as PPTA (poly(*p*-phenylene terephthalamide), used in soft body armor (SBA). These tests are frequently conducted at slow deformation rates (quasi-static) [2] relative to rates that occur in fibers during ballistic impact. To overcome this measurement challenge, the Kolsky-bar apparatus has been utilized and now allows measurement of the single fiber tensile behaviors at high strain rate (HSR) [1] deformations comparable to ballistic impact.

This study examined single PPTA fibers conducted at quasi-static conditions using two different gripping techniques with several different gauge lengths to investigate the gripping effects on the tensile tests. The test results were analysed in both parametric and nonparametric methods to investigate the distributions of the test data.

Statistical analyses were performed to 1) compare the performance of the direct and glue-tab gripping under quasi-static and HSR conditions and 2) assess several models for the data. Distributional models are useful for characterizing material properties based on distributional parameters. In addition, distributional models are often incorporated into strength models. Based on the analyses obtained by the quasi-static tests, a fiber gripping method will be developed for high strain rate test.

2 Results and Data Analysis

2.1 Strength Data

Single fiber tests have been typically conducted by using glue-tab grips with fiber lengths having a higher aspect ratio than 2000. However, HSR tests should be performed at much shorter gauge lengths in order to achieve force equilibrium during the dynamic loading. For the test with the shorter gauge lengths using the glue-tab grip, not only contributions of end effects but also the wicking of adhesives is a concern. So an alternative gripping method, the direct grip, was investigated. This method is clamping a single fiber directly and thus has no adhesive wicking.

From the quasi-static tests, we measured tensile strengths for two gripping methods (glue-tab and direct grip) at four gauge lengths (2 mm, 5 mm, 10 mm, and 60 mm). Since the strength distributions for both tests were significant, the statistical analyses were carried out and analyzed in next sections.

2.2 Non-Parametric Analysis

The gripping methods were compared graphically using kernel density [4] and quantile-quantile (Q-Q) [3] plots. More formally, two-sample Kolmogorov-Smirnov (KS) tests were conducted to see if the data can be described by a common distribution.

Kernel density plots provide a quick summary look at a univariate set of data and can show features such as: 1) the center (location) of the data; 2) the spread (scale) of the data; 3) the skewness of the data; 4) the presence of outliers; and 5) the presence of multiple modes in the data. The kernel density estimate is defined as

$$f(y) = \frac{\sum_{i=1}^{n} K\{\frac{(y-Y_i)}{h}\}}{nh} \tag{1}$$

with K, h, Y_i, and n denoting the kernel function, the window width, the i-th data point and the number of data points, respectively. The kernel density function is evaluated at a number of equally spaced locations. At a given location, the points in the sample are weighted by the kernel function and the window width to determine the estimated density at that location. The histogram is a simple kernel density estimator where h corresponds to the bin width and the sample point is either assigned full weight (if it is inside the bin) or zero weight (if it is outside the bin). Typically, however, the kernel function decays smoothly as the location y gets further from a sample point. Such a kernel density plot can show, or suggest, the underlying structure in the data more clearly than a histogram, particularly for the modest sample sizes that are often found in single fiber tests.

This study considers a Gaussian kernel function. Although many other choices are available, Silverman [4] studied the properties of various kernel functions and concluded that the kernel density plot is not overly sensitive to the choice of kernel function (he does assume that the kernel function is itself a probability density function and that it is symmetric). In particular, we used the value for h recommended by Silverman [4]

$$0.9 \min(s, IQ/1.34)\, n^{-1/5} \qquad (2)$$

with s and IQ denoting the sample standard deviation and interquartile range, respectively. The value of h controls the smoothness of the plot (larger values of h result in more smoothing). A good choice of h will balance the bias variance tradeoff. The optimal choice for h is dependent on the true underlying density function (which is the target). The value of h used here should provide near optimal performance if the underlying data is normally distributed and reasonable performance for unimodal densities that are symmetric or have moderate skewness and for densities that are moderately bimodal. Figure 1 shows kernel density plots for the 2 mm gauge length data for direct and glue-tab grips. This plot shows that the glue-tab data tend to be shorter than the direct grip data.

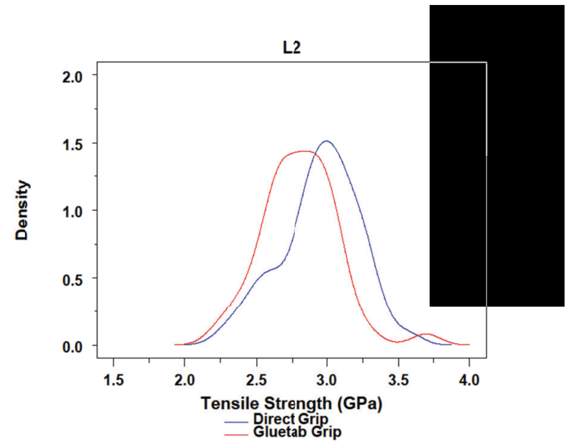


Figure 1: Kernel density plot for gauge length 2mm strength data.

Q-Q plots are used to plot the quantiles of one dataset against the quantiles of a second dataset. First, the two samples are both sorted. If the sample sizes are equal, then the i-th ordered value of the first sample is plotted against the i-th ordered value of the second sample. If the two samples are not equal, then we interpolate the values in the larger sample to create quantiles corresponding to those of the smaller sample. Q-Q plots are similar to probability plots [3]. The distinction is that in a probability plot one dataset is replaced with the quantiles from a theoretical distribution.

Q-Q plots can simultaneously show several distributional aspects of the two datasets. Shifts in location, shifts in scale, and the presence of outliers can all be detected from this plot.

If the samples come from similar distributions, the points should lie along the 45° line and the intercept, A0, and slope, A1, of a least squares line fitted to these points should be close to 0 and 1, respectively. If the points lie along a straight line that is displaced vertically from the 45° reference line, this indicates distributions with a common shape but different locations.

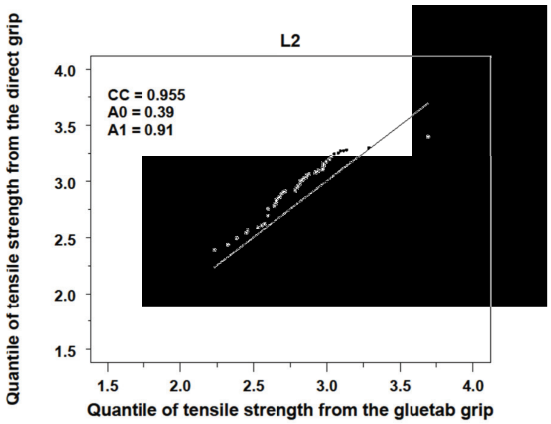


Figure 2: Q-Q plot for gauge length 2mm strength data.

Figure 2 shows the Q-Q plot for the 2 mm gauge length data. From this plot, it does not appear that the direct grip and glue-tab grip data arise from the same probability distribution. The CC value on the plot is the linear correlation coefficient of the points on the plot. The A0 and A1 values are the estimated intercept and slope of the fitted line.

We can also apply formal tests for a common distribution. One of the most often used tests for this is the two-sample Kolmogorov-Smirnov (KS) test, which is based on the statistic

$$D = \max_{-\infty < x < \infty} |EDF_1(x) - EDF_2(x)| \quad (3)$$

where EDF_1 and EDF_2 denote the empirical cumulative distribution functions of the two samples. To implement this test, we look for the maximum difference between the two empirical cumulative distribution functions. For the example shown in Figure 2, the KS test statistic is 0.312 and the 95% critical value is 0.278 so that the KS test rejects the hypothesis of a common distribution.

An advantage of Q-Q plots over the two-sample KS tests is that they show the nature of the difference between the data samples rather than just qualifying the distributions as “same” or “different”.

2.3 Distributional Fits: Parameter Estimates and Confidence Limits

Data from the quasi-static tests with longer gauge lengths have traditionally been modeled using the 2-parameter Weibull distribution. However, we should assess if the 2-parameter Weibull model also provides an adequate fit to the smaller gauge lengths. To this end, we fit 2-parameter Weibull distributions using several methods, generate confidence intervals for the parameter estimates, and assess the fit with several goodness-of-fit measures. We also consider alternative distributions.

Specifically, we compare 2-parameter Weibull, 3-parameter Weibull, normal, and *g*-and-*h* [6] distributions. The *g*-and-*h* distribution is an extension of the normal distribution that explicitly parameterizes skewness and kurtosis.

The 2-parameter Weibull distribution can be defined in terms of its cumulative distribution function

$$F(x;\gamma,L,\sigma) = 1 - e^{-L(\frac{x}{\sigma})^{\gamma}} \quad (4)$$

with γ and σ denoting the shape and scale parameters, respectively. The L parameter denotes the gauge length. Note that in the statistical literature and in most statistical software programs, the Weibull distribution is typically given without the L parameter. However, the following relationship between scale parameters used with and without the L parameter can be utilized

$$\sigma_{no\ L} = (L^{1/\gamma})\sigma \quad (5)$$

The Weibull plot is frequently used to estimate the parameters of the 2-parameter Weibull distribution. However, maximum likelihood [ML] methods [5] generally have desirable large sample statistical properties. Specifically, they become unbiased minimum variance estimators as the sample size increases and the parameter estimates have approximate normal distributions and approximate sample variances that can be used to generate confidence bounds. Note that these are asymptotic properties and how quickly the asymptotic properties take effect can vary depending on the distribution.

For the ML method, approximate confidence intervals can be obtained based on the asymptotic normality of the ML estimates (Bury [5]). More accurate limits, particularly for small samples, can be obtained by the likelihood ratio method (see Bury [5] for details).

Although the Weibull plot does not provide confidence intervals for the parameters, they can be obtained using the non-parametric bootstrap method [7, 8]. The bootstrap-based confidence intervals are obtained as follows

1. Re-sample the original data where the sampling is done with replacement and the sample is the same size as the original dataset. This is referred to as a bootstrap sample.
2. From this bootstrap sample, generate a Weibull plot to estimate the shape and scale parameters.
3. Repeat for a large number of bootstrap samples. For this study, we used 500 bootstrap samples.
4. Obtain 95% confidence intervals based on the 2.5% and 97.5% percentiles of the bootstrapped shape and scale distributions. Note that these confidence intervals may not be symmetric around the estimates.

Figures 3 and 4 summarize the parameter estimates and associated confidence intervals for the 2-parameter Weibull distributions.

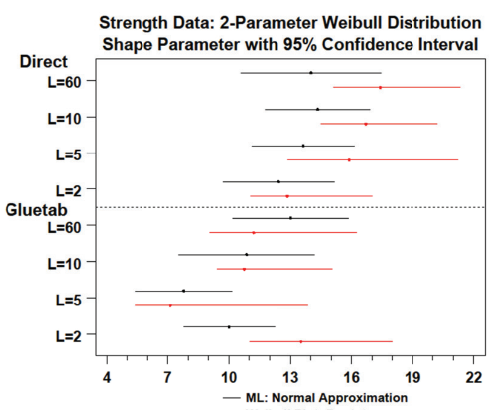


Figure 3: Confidence intervals for shape parameter for 2-parameter Weibull distribution

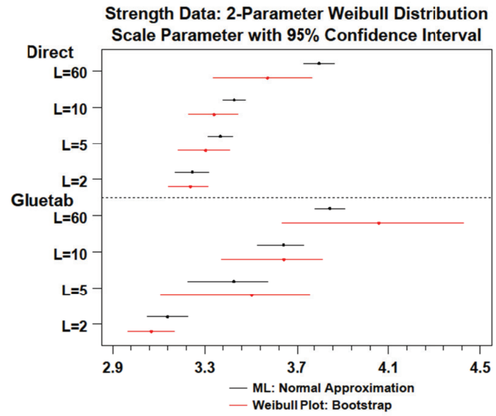


Figure 4: Confidence intervals for scale parameter for 2-parameter Weibull distribution

These plots show that the Weibull plot estimates differ from the ML estimates. In some, but not all, cases the Weibull plot estimates show greater uncertainty.

The data were also fit using normal, 3-parameter Weibull, and *g*-and-*h* distributions.

The normal distribution is fit using ML methods and the results are summarized in Figures 5 and 6.

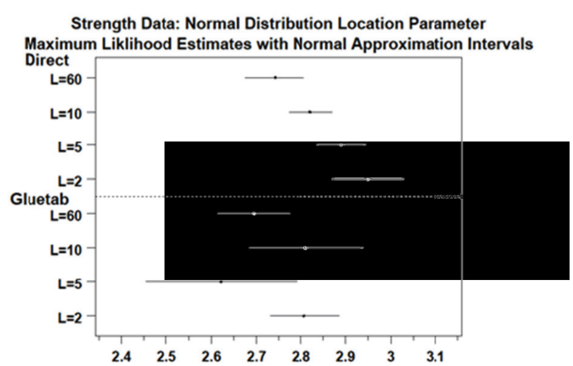


Figure 5: Confidence intervals for location parameter for Normal distribution

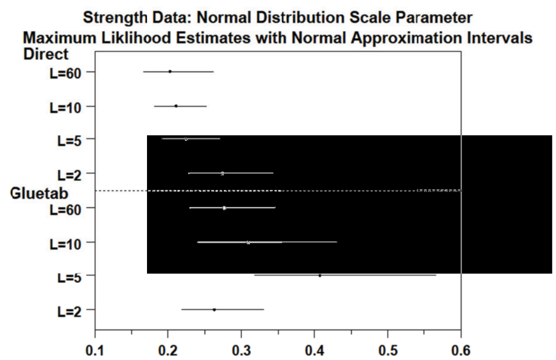


Figure 6: Confidence intervals for scale parameter for Normal distribution

These plots show that for the direct grip data, both the average strength (the location parameter) and the spread (the scale parameter) increase as the gauge length decreases. For the glue-tab data, the increasing average strength does not seem to hold for the 2 mm and 5 mm data. Also, the increasing spread does not hold for the 2 mm data. For a given value of gauge length, the direct grip data shows higher average strength than the glue-tab data for the 2 mm and 5 mm data. With the exception of the 2 mm data, the direct grip data shows smaller spread than the glue-tab data.

For the 3-parameter Weibull distribution, we fit the data using the ML method given by Bury [5]. Note that the ML estimates do not exist if the shape parameter is less than 1 and the parameters have infinite variance when the shape parameter is less than 2. For this reason, we investigated several alternative fitting methods (there are a number of other methods not discussed here). In particular, we compare the ML estimates to the probability plot correlation coefficient (PPCC) [3] method.

The PPCC method is based on the following two ideas.

1. The straightness of the probability plot is a good measure of distributional fit.
2. The correlation coefficient of the points on the probability plot is a direct assessment of the straightness (linearity) of the probability plot.

The probability plot used here is formed by plotting the sorted data on the y-axis and the order statistic medians for the desired distribution on the x-axis. That is,

$$X(i) = G(U(i))$$

G denotes the percent point function (= the inverse of the cumulative distribution) of the distribution to be tested and the uniform order statistic medians are computed as

- $U(n) = 0.5^{(1/n)}$
- $U(1) = 1 - U(n)$
- $U(i) = (i - 0.3175)/(n + 0.365)$ for i = 2, 3, …m…, n-1

Probability plots formed in this way have the property that they are invariant to location and scale. In practical terms, this means the linearity of the probability plot is independent of the values of the location and scale parameters. In addition, the intercept and slope of the line fitted to the points on the probability plot provide estimates for the location and scale parameters, respectively.

If the shape parameter of the 3-parameter Weibull distribution is to be estimated, the PPCC method is implemented in two plots. The first plot is generated by varying the value of the shape parameter on the x-axis. For each value of the shape parameter, the correlation coefficient of the associated probability plot appears on the y-axis. The estimate of the shape parameter is the one that results in the maximum correlation coefficient. Based on this value of the shape parameter, a final probability plot is generated. The location and scale estimates are the intercept and slope of a least squares line fitted to the points on the probability plot. If the shape parameter is not fitted, but instead set from the beginning, then only a single probability plot is needed. Confidence intervals can be obtained via a bootstrap approach. An example of the PPCC/probability plot method for the direct grip gauge length 2 mm case is given in Figures 6 and 7.

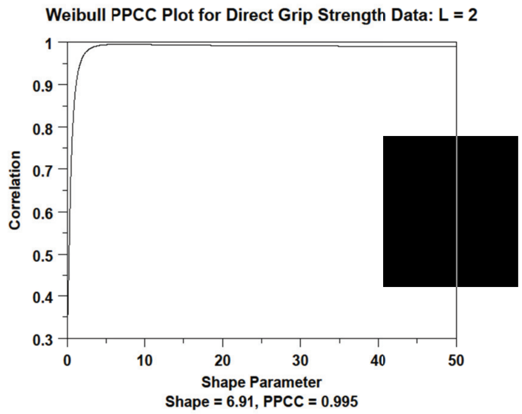


Figure 6: 3-Parameter Weibull PPCC plot for direct grip strength data for 2 mm gauge length

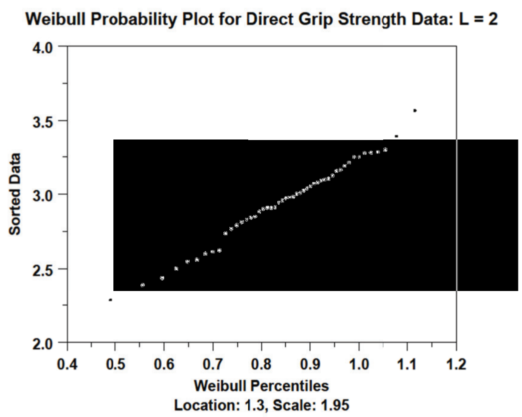
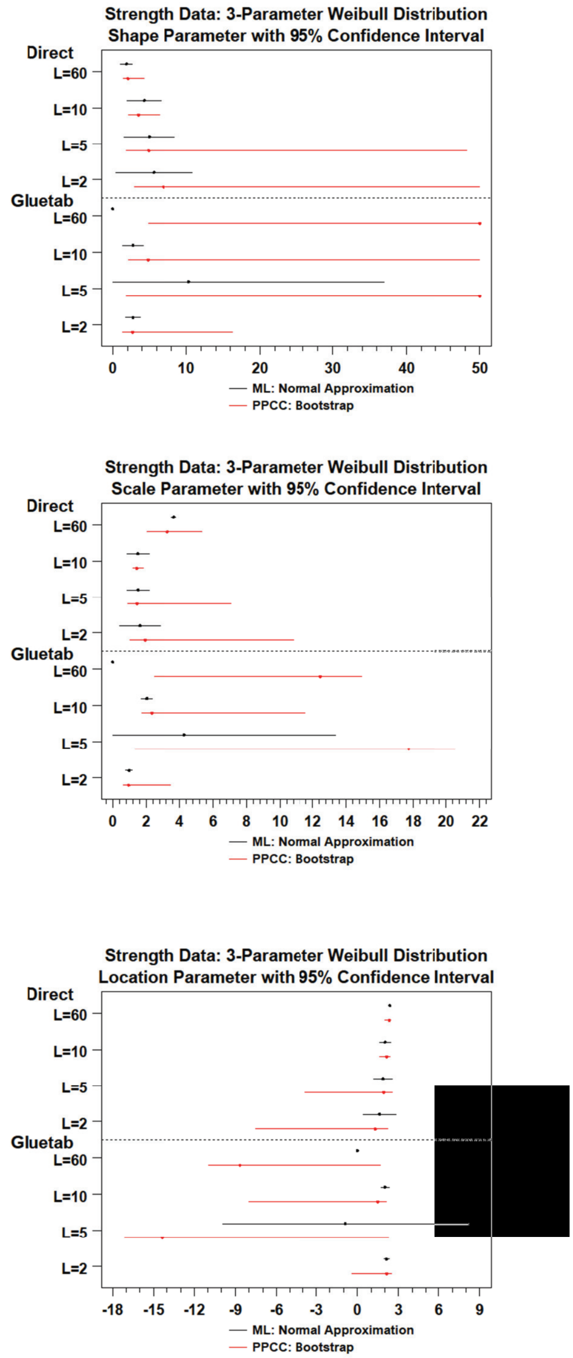


Figure 7: 3-Parameter Weibull probability plot for direct grip strength data for 2 mm guage length

Although the PPCC method is similar to the Weibull plot method, there are a few distinctions. The primary difference is that the Weibull plot is used for a 2-parameter Weibull while the PPCC method fits a 3-parameter Weibull distribution (this is due to the invariance of the probability plot to location and scale). The PPCC method is generic and can be applied to many other distributions while the Weibull plot is restricted to the 2-parameter Weibull distribution. The PPCC method provides an objective measure of goodness of fit (i.e., the PPCC value).

Figures 8-10 summarize the estimates and confidence intervals for the 3-parameter Weibull.



Figures 8-10: Confidence intervals for 3-parameter Weibull distribution

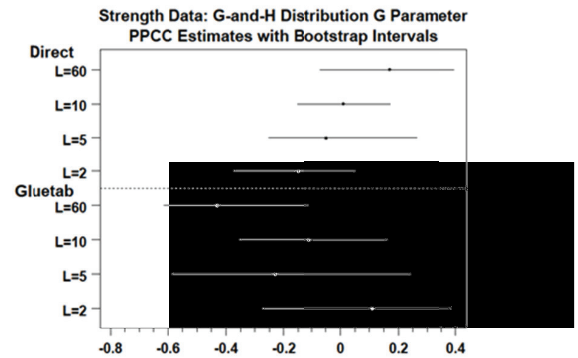
One signature of the PPCC method for the 3-parameter Weibull distribution is that if the underlying distribution is actually Gumbel, the PPCC plot will indicate an asymptotic value of the shape parameter (50 in these plots, but that is an arbitrary cut-off). When the PPCC method indicates 50 (or whatever value is used for the upper limit) for the value of the shape parameter, the data should probably be modeled by a Gumbel distribution. Likewise, when the confidence interval for the shape parameter extends to 50, there is evidence of Gumbel behavior. Note that the ML method failed for the glue-tab 60 mm data.

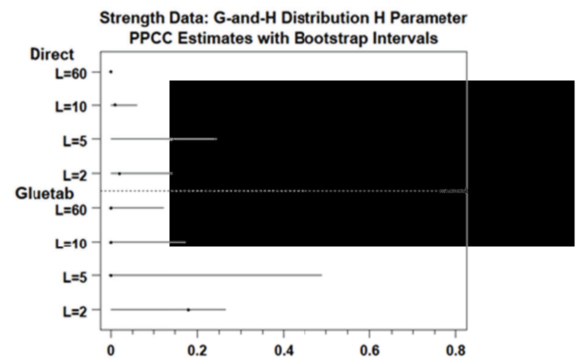
The g-and-h distribution [6] is defined in terms of its percent point function

$$G(p; l, s, g, h) = l + s\,\frac{(e^{g z_p} - 1)e^{h z_p^2}}{g} \qquad (6)$$

The z_p term is the percent point function (inverse CDF) of the standard normal distribution. The l and s parameters are the location and scale, respectively. The g parameter controls the skewness and can take on values between -1 and +1 with a value of 0 indicating symmetry. The h parameter controls the kurtosis (i.e., the "heavy tailedness") and can take on values between 0 and 1. A value of 0 indicates kurtosis equivalent to a normal distribution and a value of 1 indicates kurtosis equivalent to a Cauchy distribution. When g and h are both 0, the g-and-h distribution is a normal distribution.

The g-and-h distribution is fit using the PPCC method with confidence intervals determined with the bootstrap method. Summary plots for the g and h parameters are given in Figures 11 and 12 (the plots for the location and scale parameters are similar those for the normal distribution). The point estimates show that the h parameter is near zero except for the direct grip 5 mm and the glue-tab 2 mm datasets. In addition, the g parameter for the direct grip shows a consistently decreasing value (and changing from positive to negative skewness). The glue-tab data, with the exception of the 5 mm dataset, shows a trend in the opposite direction. However, these observations need to be tempered by the high variability exhibited by both the g and h parameters. These parameters are based on third and fourth order moments which can be highly influenced by a few extreme points in the tail.





Figures 11-12: Confidence intervals for *g* and *h* parameters of the *g*-and-*h* distribution

2.4 Distributional Fits: Assessing Goodness of Fit

The primary analytical tool used for assessing distributional goodness-of-fit was the Anderson-Darling (AD) test. The AD test involves a comparison of the empirical cumulative distribution function to a theoretical distribution function. It is a refinement of the Kolmogorov-Smirnov (KS) goodness-of-fit test that is more sensitive than the KS test to differences in the tails of the distribution. It is also has more power than the KS test. The AD test statistic is

$$A^2 = -n - \sum_{i=1}^{n} \frac{2i-1}{n}\left\{\ln\left(F(Y_i)\right) + \ln\left(1 - F(Y_{n+1-i})\right)\right\} \qquad (7)$$

with F denoting the cumulative distribution function of the theoretical distribution. The critical values for this test are obtained via simulation.

Figures 13 and 14 compare the goodness-of-fit for the various methods for the 2-parameter and 3-parameter Weibull distributions. Figure 15 compares the goodness-of-fit between the normal and the g-and-h distributions. For the AD test, a smaller value indicates better goodness-of-fit.

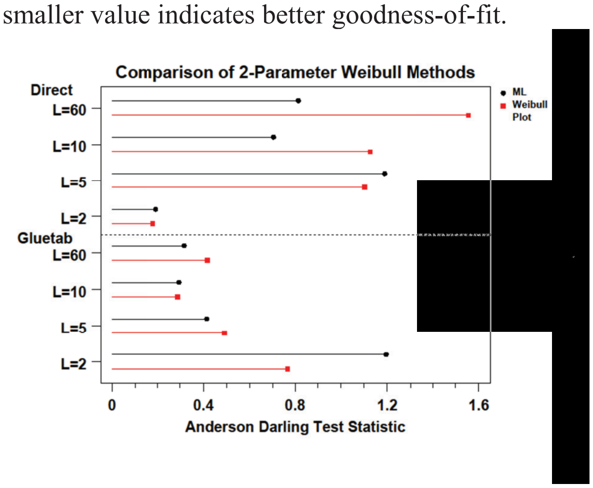


Figure 13: Anderson-Darling values for the 2-parameter Weibull distribution

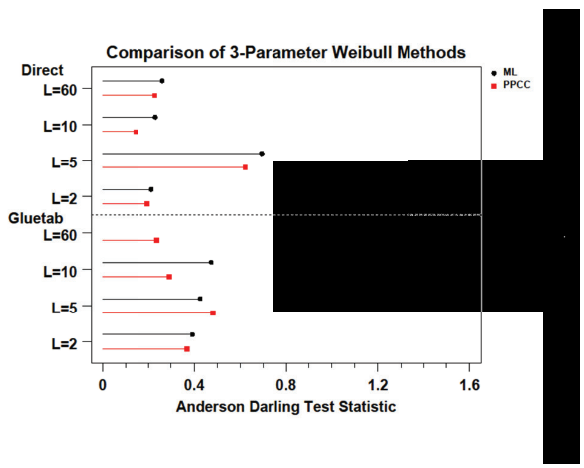


Figure 14: Anderson-Darling values for the 3-parameter Weibull distribution

For the 2-parameter Weibull, with the exception of the glue-tab 2 mm data, the goodness-of-fit is either comparable or better for the ML method. For the 3-parameter Weibull, the ML and PPCC generally have comparable goodness-of-fit.

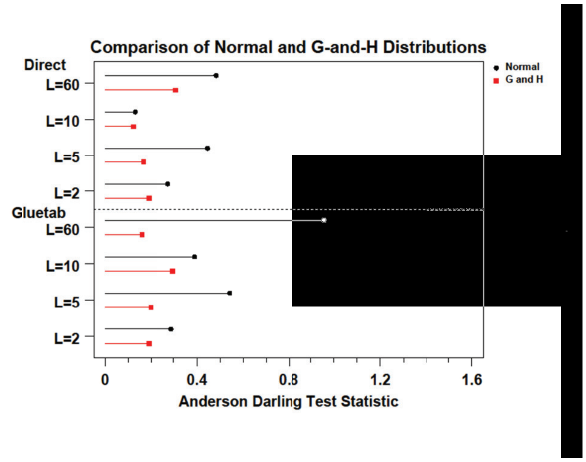


Figure 15: Anderson-Darling values for the normal and the g-and-h distributions

Figure 15 shows that, as expected, the g-and-h distribution provides better goodness-of-fit than the normal distribution. In comparing these to the g-and-h parameter estimates in Figures 11 and 12, the cases that show the most significant improvement in goodness-of-fit correspond to the cases where either the g or the h parameter (or both) is not close to zero.

In addition to providing parameter estimates, the Weibull plot can also provide a graphical assessment of goodness-of-fit for the 2-parameter Weibull distribution. Probability plots also provide a graphical assessment of goodness of fit. However, they are more generally applicable than the Weibull plot in that they can be applied to any distribution and therefore allow comparisons between different distributions. The PPCC value associated with the probability plot can also be used to compare the fits from different probability distributions. Figure 16 shows an example of the probability plots for the glue-tab 2 mm data for the four different distributions investigated here.

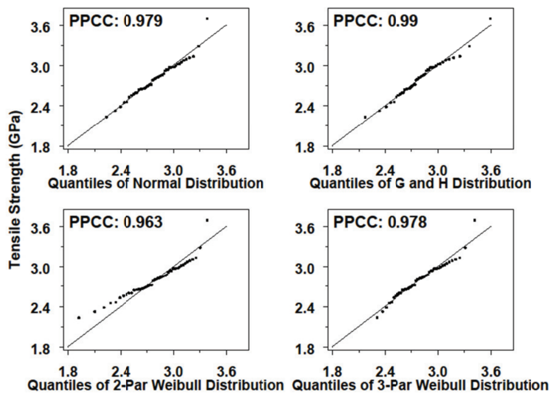


Figure 16: Probability plots for the glue-tab grip at 2 mm gauge length

3 Concluding Remarks

We have compared the single fiber tensile strengths using direct grip and glue-tab grip at various gauge lengths using graphical methods. We have compared the fits based on conventional 2-parameter Weibull models with several alternative distributional models.

This investigation showed that the behavior for the direct gripping data is different than for the glue-tab data. In some cases, we can obtain better goodness-of-fit over the 2-parameter Weibull distributions by using either 3-parameter Weibull or *g*-and-*h* distributions. However, the parameter estimates for these distributions have more uncertainty than do the parameter estimates for the 2-parameter Weibull distribution.

Similar analysis is being applied to the failure strain data and eventually to high strain rate data collected using a Kolsky bar.

References

[7] Kim, JH, Heckert, NA, Leigh, SD, Rhorer, RL, Kobayashi, H, McDonough, WG, Rice, KD, Holmes, GA. Statistical analysis of PPTA fiber strengths measured under high strain rate condition. *Composites Science and Technology* (10 1016/j Compscitech 2012 03 021) 2012.

[16] Kim, JH, Holmes, GA, Leigh, SD, Kobayashi, H, McDonough, KMcDonough, WG, Rice, KD, Holmes, GA. Effects of fiber gripping methods on the single fiber tensile test: I. Non parametric statistical analysis. *Journal of Materials Science* 2013;48:3623-3637.

[3] NIST/SEMATECH e-Handbook of Statistical Methods, http://www.itl.nist.gov/div898/handbook/eda/section3/qqplot.htm, probplot.htm, ppccplot.htm, April, 2012.

[4] Silverman "*Density estimation for statistics and data analysis*". Chapman and Hall, 1986.

[5] Bury "*Statistical distributions in engineering*". Cambridge University Press, 1999.

[6] Hoaglin "Summarizing shape numerically: The g-and-h distributions", chapter 11 in "*Exploring data tables, trends, and shapes*". Eds. Hoaglin, Mosteller, and Tukey, Wiley, 1985.

[7] Efron and Tibshirani "*An Introduction to the Bootstrap*". Chapman & Hall/CRC, 1993.

[8] Efron and Gong “A leisurely look at the bootstrap, the jackknife, and cross-validation”, *The American Statistician*, February, 1983.

[9] Cohen and Whitten “*Parameter Estimation in Reliability and Life Span Models*”. Marcel Dekker, 1988.