# An Iterative Method to Estimate Grain-size Distribution from Soil-water Characteristic Curve

Minh Nguyen, David Elwood
*Department of Civil, Geological and Environmental Engineering – University of Saskatchewan, Saskatoon, Saskatchewan, Canada*

## ABSTRACT
Design of an effective capillary break requires knowledge of the soil water characteristic curve (SWCC) for a given soil. Numerous methods for predicting the unsaturated properties (SWCC) and unsaturated permeability based on basic soil parameters have been introduced to reduce the cost of unsaturated soil testing. The current research proposes another unsaturated soil estimation method that uses a predetermined soil-water characteristic curve to estimate the grain-size distribution (GSD) using computer iteration. The results indicated that it was possible to back-calculate a GSD from a given SWCC as well as a potential way to determine different combinations of grain-size to produce the same SWCC. A Monte-Carlo approach examining the variations to the GSD and the associated packing porosity are provided. Results are presented for a silty sand indicating a strong correlation with the actual SWCC and GSD.

## RÉSUMÉ
La conception d'une rupture capillaire efficace nécessite la connaissance de la courbe caractéristique de l'eau du sol (SWCC) pour un sol donné. De nombreuses méthodes de prédiction des propriétés insaturées (SWCC) et de la perméabilité insaturée basées sur des paramètres de base du sol ont été introduites pour réduire le coût des essais de sol non saturé. La recherche actuelle propose une autre méthode d'estimation des sols non saturés qui utilise une courbe caractéristique sol-eau prédéterminée pour estimer la distribution granulométrique (GSD) à l'aide d'une itération informatique. Les résultats ont indiqué qu'il était possible de rétrocalculer un GSD à partir d'un SWCC donné ainsi qu'un moyen potentiel de déterminer différentes combinaisons de granulométrie pour produire le même SWCC. Une approche de Monte-Carlo examinant les variations du GSD et la porosité de garnissage associée est fournie. Les résultats sont présentés pour un sable limoneux indiquant une forte corrélation avec le SWCC et le GSD réels.

## 1 INTRODUCTION

Unsaturated soil mechanics has been developed significantly over the years and implemented to solve numerous geotechnical problems. The cost of performing direct measurement of unsaturated soil properties, is often excessive and not readily available in most labs. This has led to the pursuit of new means of predicting unsaturated properties based on basic, easily measured soil properties. There has been considerable research that attempts to evaluate the soil water characteristic curve (SWCC) based on a soil's grain size distribution (GSD) and basic mass – volume relationship with reasonable results. Because the matric suction of a given soil is controlled by the pore-size distribution and not actually by the GSD, the use of GSD to determine an accurate SWCC has been elusive.

This research demonstrates that a back analysis method of predicting a GSD for a given SWCC might be advantageous. Capillary break layer, for example, would benefit from reverse engineering a soil from a designer SWCC, perhaps further optimizing the performance of the layer. Capillary break occurs in unsaturated conditions when in a fine-grained soil when it overlies a coarse-grained soil. The SWCC of the coarse-grained soil was determined to be one major factor that influences the expected water storage capacity of the upper clay layer. Proper selection to build the capillary break layer will maximize the performance of the upper clay barrier ability to limit infiltration towards lower depths (Zornberg, Bouazza and McCartney 2010). The back analysis method could potentially bypass the arduous phase of testing multiple soils to find a suitable SWCC as it can take in a desired SWCC and estimate a suitable GSD.

## 2 LITERATURE REVIEW

Methods to predict the SWCC from a given GSD and basic mass – volume properties are generally categorized in three categories:
- Statistical estimation of water content at selected matric suction values (Gupta and Larson 1979).
- Correlation by regression analysis of soil properties with the fitting parameters of an analytical equation used to represent the SWCC (Perera, et al. 2005, Vanapalli and Catana 2005).
- Physico – empirical based concept model to estimate the SWCC (Arya and Paris 1981, Fredlund 2000)

The first method involves relating water content to basic soil properties at a selected matric suction value. This evaluation is generally performed with regression analysis followed by curve fitting to an experimentally determined SWCC. The second method correlates basic soil properties to fitting parameters of an equation that represents the

SWCC by regression analysis. The third method works under the assumption that the radius of a soil particle can be correlated to the typical pore radius. In other words, the method converts a GSD to pore-size distribution, which is then related to water holding capacity of a soil and the negative pore pressure derived from capillary theory.

The physico-empirical method is the focus of this research. The method described by Arya and Paris (1981) predicts a SWCC by using the measured GSD, bulk density data, and void ratio. The radius of each measured particle size fraction were used to determine the equivalent pore volume and a pore radius of each respective grain size fraction. The pore volume determines the amount of water held in the pores while the pore radius is used to determine the matric suction using capillary theory. Progressive accumulation of the fractional pore volumes results in the volumetric water content of the soil at each suction stage.

Another physico-emperical method was conducted by Fredlund (2000). Fredlund (2000) was based on three fundamental theorems:

- Each uniform and homogeneous particle size that composed a soil would have a unique drying curve.
- The capillary model is best suited for estimation of the air entry value (AEV) of each collection uniform and homogeneous particle size.
- The sum of each unique SWCC would result in the SWCC of the soil composed of uniform and homogeneous particle sizes.

The method proposed by Arya and Paris (1981) assumed that when the soil is divided into smaller fractions, particles in each fraction is in a discrete domain and when all domains are assembled, the resulting assemblage has the same bulk density as the natural soil. However, in a natural soil sample, particles are not packed in discrete domains consisting of uniform-size particles but randomly distributed in soil. The assumption made by Arya and Paris (1981) does not account for a more realistic structure that smaller particles can fall into and reduce the effect larger pores which, was accounted for in Fredlund (2000). The Fredlund (2000) method was used as the basis for this research due to the inherent ability to adjust the particle packing to overcome the limitations presented in the Arya and Paris (1981) research.

Fredlund (2000) first fitted the experimental GSD to generate a continuous equation for the GSD. The GSD equation was represented by three parameters: $a_{gr}$, $n_{gr}$, and $m_{gr}$. The GSD was divided into smaller fractions and corresponding Fredlund – Xing (1994) SWCC curve fit parameters ($a_f$, $n_f$, and $m_f$) were determined for each fraction. The pore volume of each smaller fraction was determined using the corresponding weight fraction and packing porosity. This packing porosity accounted for the shape of the particle and how it influences the packing structure of the soil. Finally, the SWCC was determined by summing the pore volume fractions, along with the corresponding Fredlund – Xing (1994) curve fit parameters, until the summed pore volume reached the in-situ porosity of the soil. This summation to the in-situ porosity accounted for the effect of smaller particles falling into bigger voids. The summation of each unique SWCC of each grain size fraction up to this point was the resulting SWCC estimation of the soil sample

## 3 METHODOLOGY

### 3.1 The modified Fredlund method

A new SWCC prediction method using GSD based on the basis of Fredlund (2000) due to Fredlund's assumption to address for a more realistic soil structure. For clear transparency, at the time of research, the modified Fredlund was created based on the understanding of the author of this paper of Fredlund (2000). It was discovered near the end of the project that this method was different compared to Fredlund (2000). This method is still heavily based on the concepts of Fredlund (2000) and therefore was called the modified Fredlund method.

The discussion on the differences between the modified Fredlund method and Fredlund (2000) was detailed in Nguyen (2022). This section only includes a short summary was what done differently in the modified Fredlund method.

The packing porosity, $n_p$, was treated as an extra 'curve-fit' parameter with a range between 0.5 – 1; the factor could then be iteratively solved for, using the Python curve-fit feature. The range 0.5 – 1 was selected was because SWCCs generated using $n_p$ values below 0.5 did not change relative to that of an $n_p$ = 0.5. Therefore, an $n_p$=0.5 is considered a lower bound. Correlations of $n_p$ to readily measured soil properties was attempted. Given the dependence on soil porosity, it was thought that assessing $n_p$ relative to the relative density, $D_r$ might be possible. However, $D_r$ was concluded to be inadequate as the parameter could not account for the extremities of $n_p$ range.

Fredlund (2000) explained that a soil's AEV is approximately equal to the $a_f$ parameter, and therefore the AEV should be used as an estimate for $a_f$. The original suggested that AEV should be estimated based on capillary theory. However, to use capillary theory, pore radius of each soil fractions is required. Fredlund (2000) did not elaborate how this pore radius is calculated. To fill in the gap of knowledge of the author, other research were consulted. Sakaki et al. (2014) conducted research to empirically relate the AEV with characteristic particle diameters ($D_{10}$, $D_{30}$, $D_{60}$, ..., $D_{90}$) in sandy soils. Results determined in this research showed that, contrary to capillary theory which suggested that the AEV would be influenced by larger pore sizes, the effect of smaller particles filling larger pores had a major impact on the influence of the larger pores on the water retention properties of the soil. The findings of Sakaki el al. (2014) with respect to particle interaction and pore volume was consistent with those reported by Fredlund (2000). Sakaki et al. (2014) determined that $D_{30}$ and $D_{50}$ showed the highest correlation to AEV with $R^2$ of 0.975 and 0.925 respectively. The correlation of $D_{30}$ and $D_{50}$ to AEV take the following forms:

$$AEV = 8.2D_{30}^{-0.99} \quad \text{for } C_u < 5.6 \tag{1}$$

$$AEV = 9.5D_{50}^{-1.05} \quad \text{for } C_u < 3.0 \tag{2}$$

For the estimation of $n_f$ and $m_f$ of each grain size fraction, the author of this paper first calculated an effective grain size diameter, $d_e$ for the soil sample being investigated. An overall $n_f$ and $m_f$ were calculated based on the previous calculated $d_e$. The fractional $n_f$ and $m_f$ of each grain size were determined by dividing the previously calculated overall $n_f$ and $m_f$ accordingly to the probability distribution of each grain size fraction to represent the individual SWCC.

### 3.2    Coding Methodology

To achieve the goal of predicting a GSD from a given SWCC, a Python curve fit function (non-linear least square method) was utilized. Two requirements needed to be satisfied before this function can be used:
-    A SWCC prediction function that can take in GSD and basic soil properties input
-    A data set of a predetermined SWCC.

It is important to understand that the Python curve fit function by itself is only a statistical analysis tool. The modified Fredlund function took in GSD curve fit parameters acquired from Fredlund's unimodal GSD equation, the packing porosity, $n_p$, and basic soil properties (specific gravity and bulk density) as the inputs. The constructed modified Fredlund function was then provided to the curve fit function. When a predetermined SWCC is given, the curve fit function will iteratively change the inputs (except for bulk density and specific gravity) of the modified Fredlund function to minimize the squared difference between desired and calculated SWCCs. The inputs of the modified Fredlund function are reported as the back calculated GSD.

The bulk density and specific gravity inputs of the Fredlund function were left intentionally as constant values and therefore, these properties are not iteratively changed in the back analysis program. In instances where the specific gravity and bulk density of the soil are specified values, those terms can be directly inputted into the model. Conversely, if the specific gravity and bulk density are unknown, then the designer can use suitable assumed values for these properties. The back analysis program will be able to calculate a GSD based on the constant values. By leaving these inputs as constant values, it will also reduce the iteration time of the back analysis program.

### 3.3    Boundary conditions

Boundary conditions were required for the curve fitting process. Without the boundaries (as in any model), the iteration would result in an infinite number of grain sizes and unable to converge to a unique solution.

GSD data of 23 soils were acquired from published literature. The primary focus of the published data was on soils comprised of silty sands. The data of these published soils was published in Nguyen (2022). Fredlund's unimodal GSD equation was used to determine the GSD parameters of the collected data. The ranges for the GSD parameters were 0.12 – 1.9, 1.09 – 10, and 0.503 – 1.9 for $a_{gr}$, $n_{gr}$, and $m_{gr}$ respectively.

When determining the different GSDs producing matching SWCCs, the back analyzed GSDs were used to predict their respective SWCC. A statistical analysis was conducted to compare the predicted SWCCs and the recorded SWCC of the tested soil. SWCCs with $R^2 < 0.98$ were excluded.

### 4    MATERIAL TESTING

The material used for this research is a sand obtained from road construction in Clavet, Saskatchewan. The soil is light gray in colour and is classified as a poorly graded sand (SP). The content of the soil is: 0.9% medium sand, 84% fine sand, 10% silt, and 5.1% clay sized particles. The GSD and SWCC of the soil were also determined which could are shown on Figure *1* and Figure *2*. The recorded SWCC data were curve – fitted using the Fredlund – Xing (1994) equation. The recorded GSD was also curve – fitted using Fredlund (2000) equation. The curve fit parameters could be seen on their respective figure. Note that $a_f$, $n_f$, and $m_f$ denoted the curve fit parameters for SWCC while $a_{gr}$, $n_{gr}$, and $m_{gr}$ denoted the curve fit parameters GSD. Table 1 shows the basic properties of the soil for the analyses.
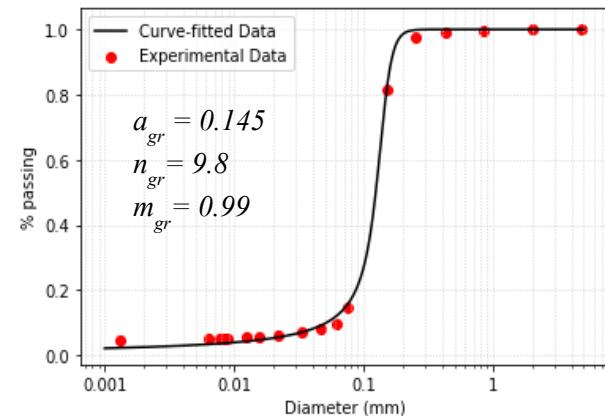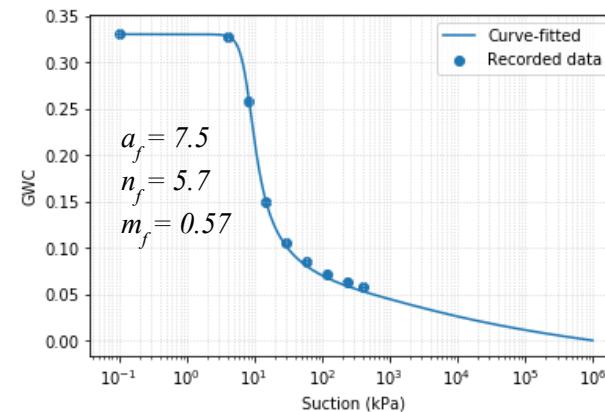


Figure 1: Experimental GSD of Clavet sand



Figure 2: Experimental SWCC of Clavet sand

Table 1: Basic properties of Clavet sand

| Basic properties | Value |
|---|---|
| Bulk density (kg/m$^3$) | 1670 |
| Specific gravity, $G_s$ | 2.67 |
| Porosity | 0.57 |
| $D_{60}$ (mm) | 0.13 |
| $D_{10}$ (mm) | 0.05 |

## 5    RESULTS AND DISCUSSION

### 5.1    The modified Fredlund method

As mentioned previously, the modified Fredlund method was constructed as a computational function to predict the SWCC from GSD. The $C_u$ of the Clavet sand was determined to be 2.2 which satisfied the condition to use both AEV correlations using $D_{30}$ and $D_{50}$ from Sakaki et al. (2014). Figure 3 presented the predicted SWCCs using $D_{30}$ and $D_{50}$ to estimation for $a_f$.
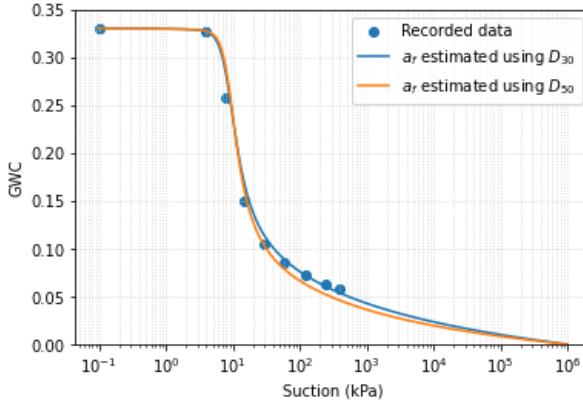


Figure 3: Estimated SWCCs using modified Fredlund method

The $n_p$ value for the Clavet sand was determined to be 0.78. The predicted SWCCs using both $a_f$ correlations of  Sakaki et al. (2014) produced good fit with R$^2$ value of 0.99 determined for both data when compared with the SWCC of the Clavet sand. The parameters of the predicted SWCC with $a_f$ estimated from $D_{30}$ are: $a_f$ = 7.9, $n_f$ = 5.3, $m_f$ = 0.53, and $n_p$ = 0.78. The parameters of the predicted SWCC with $a_f$ estimated from $D_{50}$ are: $a_f$ = 8.3, $n_f$ = 5.7, $m_f$ = 0.57, and $n_p$ = 0.78. The parameters of both predicted SWCCs are approximate similar to the curve fit parameters of the experimental data ($\underline{a_f}$ = 7.5, $n_f$ = 5.7, and $m_f$ = 0.57). The results in the next following sections were conducted using $a_f$ correlation using $D_{30}$.

### 5.2    Sensitivity analysis

A sensitivity analysis using the Monte Carlo approach was conducted to determine the effect of GSD curve fit parameters ($a_{gr}$, $n_{gr}$, and $m_{gr}$) and $n_p$ on the outcome of the computational method. The published data of silty sands were used to generate a normal probability distribution for each GSD curve fit parameters (Table 2). A separate Python function to filter the randomly generated values

were created as using the probability distribution created negative values which is not possible for a GSD curve fit parameter. Due to the lack of data to generate a probability distribution for $n_p$, the parameter was simply varied from 0.5 – 1 to demonstrate the effect. Due to the large amount of data generated from a Monte Carlo approach, a few data set were manually selected to demonstrate the results.

Table 2: Mean and standard deviation of each GSD curve fit parameter based on collected data of silty sand

| Parameter | Mean (μ) | Standard deviation (σ) |
|---|---|---|
| $a_{gr}$ | 0.43 | 0.42 |
| $n_{gr}$ | 4.67 | 2.66 |
| $m_{gr}$ | 1.12 | 0.39 |

As shown in Figure 4 and Figure 5, varying the $a_{gr}$ parameter resulted in a lateral shift of the SWCC, which resulted in a change of AEV. However, this did not mean that $a_{gr}$ is correlated to AEV. Varying $a_{gr}$ also results in a lateral shift of the entire GSD. The slope of the GSD represents the dominant particle sizes, meaning that when the entire GSD is shifted laterally, the dominant particle sizes are changed. Smaller $a_{gr}$ suggests a smaller representative or controlling particle size. This in turn results in smaller pore sizes and a shift of the SWCC to the right side (higher suction for a given water content) and vice versa.
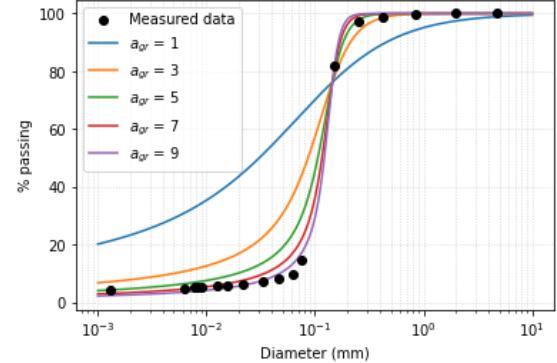


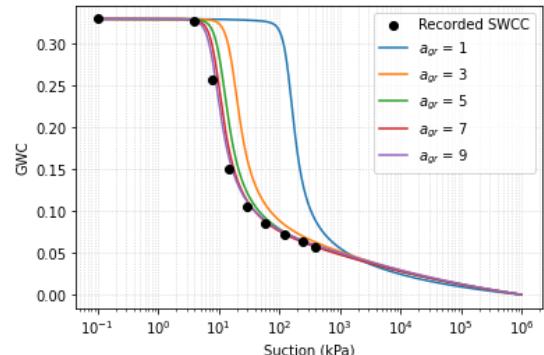Figure 4: Resulting GSDs by varying $a_{gr}$ while holding other parameters constant



Figure 5: Resulting SWCCs by varying $a_{gr}$ while holding other parameters constant

Varying $n_{gr}$ and $m_{gr}$ also shifted the SWCC laterally (Figure *6* to Figure *9*). In the case of varying $n_{gr}$, it was expected that it would change the slope and the approach to residual of the SWCC. For example, a shallow slope would indicate a more well graded soil which also indicated a more diverse pore size. However, the result shown in Figure *7* did not reflect this expectation. The result showed that a more well graded soil would result in a higher AEV due to the higher fines content. The same result could be seen for varying $m_{gr}$ (Figure *9*); a higher fines content only results in change of AEV with no change in the overall shape of the SWCC.
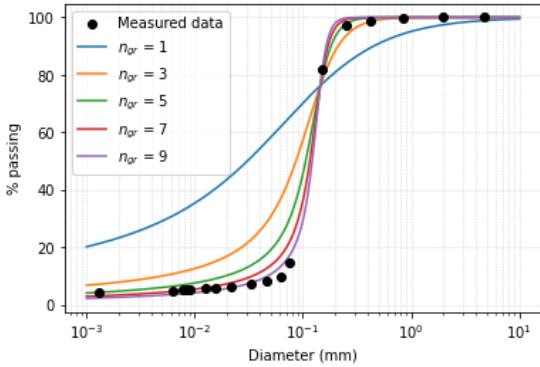


Figure 6: Resulting GSDs by varying $n_{gr}$ while holding other parameters constant
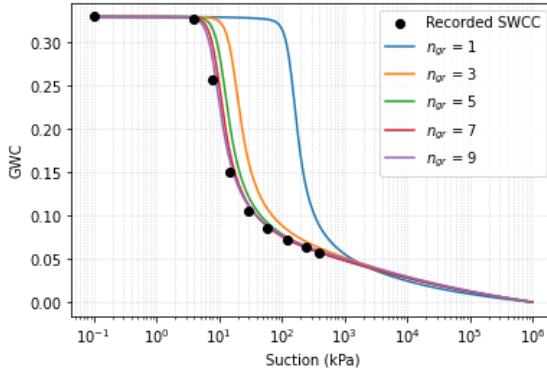


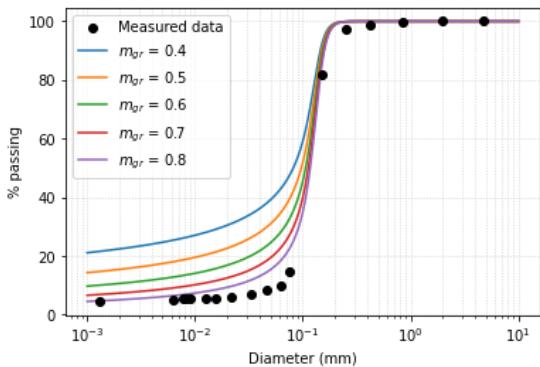Figure 7: Resulting SWCCs by varying $n_{gr}$ while holding other parameters constant



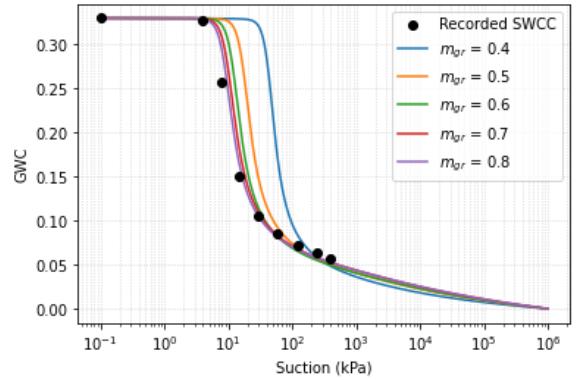Figure 8: Resulting GSDs by varying $m_{gr}$ while holding other parameters constant



Figure 9: Resulting SWCCs by varying $m_{gr}$ while holding other parameters constant

Figure *10* shows the result from varying $n_p$ while holding GSD curve fit parameters constant. Figure *11* shows the corresponding SWCCs when varying $n_p$ while holding the GSD parameters constant. The result shows that varying $n_p$ changes the overall shape of the SWCC with no discernable change of AEV. The curve generated by using an $n_p = 0.99$ seems to suggest that the AEV was increased. However, a change in AEV was not possible and in fact the shape of the SWCC simply masks the AEV because the desaturation slope of the SWCC became extremely shallow and the approach to residual became steep due to the increased water retention capacity from the soil being in a denser state. This is because for the modified Fredlund method, the AEV is estimated using characteristic particle diameters and is not a function of the packing porosity. As the GSD curve fit parameters, which defined the shape of the GSD curve, were held constant for this analysis, $D_{30}$ or $D_{50}$ would not have been changed and therefore the AEV cannot change.

The packing porosity, $n_p$, represents the porous fractional volume created from the shape and arrangement of soil particles (Smith, Foote and Busang 1929). Since $n_p$ represents the porosity, it was expected that lower $n_p$ value, would result in smaller pores that in turn, increase the water retention capacity and vice versa. Figure *11* shows that as $n_p$ increases, the desaturation slope becomes shallower and the approach to the residual becomes steeper. This is an indication of a higher water retention capacity. The results are contrary with the expectation based on the definition of packing porosity. Considering this, it is possible that the packing porosity may not be a suitable parameter to use for the calculation of pore volume. Instead, the atomic packing factor (APF), which is defined as the fraction of volume occupied by solid particles, would be more appropriate since it would be able to describe the calculated results. If $n_p$ represents the APF, increasing $n_p$ results in higher water retention capacity from a more densely packed structure which decreases the pore sizes and allow for a higher capillary action and vice versa.
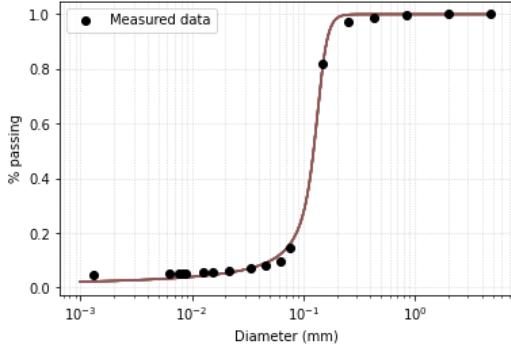
Figure 10: Resulting GSD from varying $n_p$ while holding GSD parameters constant
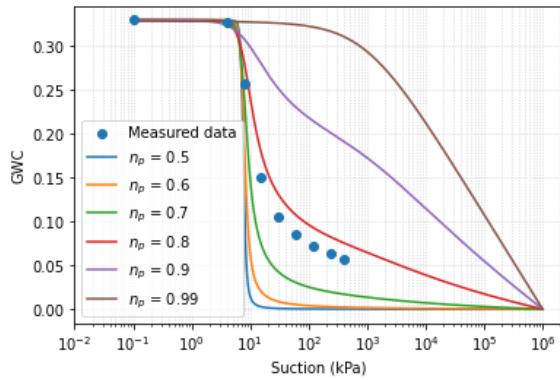


Figure 11: Resulting SWCCs from varying $n_p$ while holding GSD parameters constant

## 6    ESTIMATING GSD FROM A GIVEN SWCC

With the modified Fredlund method constructed, the modified Fredlund function was provided to Python curve fit function to back analyze the GSD. The back calculated parameters were 0.33, 4.8, 0.67 and 0.78 for $a_{gr}$, $n_{gr}$, $m_{gr}$ and $n_p$ respectively. As shown in Figure *12*, the back calculated GSD did not agree with the measured GSD data. Two scenarios were possible for the discrepancies observed between the two set of data. The first possible case was that there were errors associated with the original Fredlund (2000) model that were carried forward to the modified method. The second scenario would simply be that the function was able to find a solution that satisfied the end condition which was to determine a GSD that produced a SWCC similarly to the initially given SWCC.
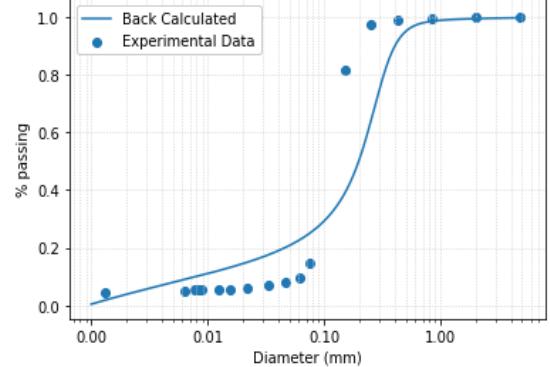


Figure 12: Comparison between back calculated GSD and recorded GSD data.

To test these hypotheses, the modified Fredlund method was used to predict the SWCC of the back calculated GSD. The resulting SWCC fitted well ($R^2 = 0.99$) with the recorded data (Figure *13*), confirming that the discrepancies observed between two sets of GSD data to the latter case – more than one possible solution exists.
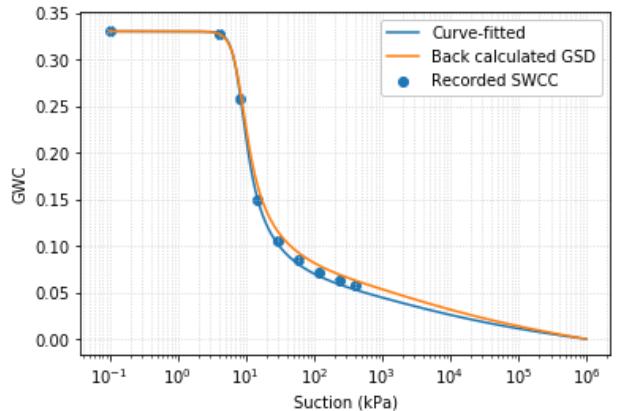


Figure 13: Comparison between SWCC predicted using back calculated GSD and recorded SWCC data.

Based on the finding that several solutions may exist, it was believed that there might be more than one possible GSD that produce similar SWCC. To determine this likelihood, the SWCC to GSD iterative method was modified to accommodate a Monte Carlo approach. 1500 sets of GSD curve fit parameters and $n_p$ were back calculated and then used to predict the corresponding SWCCs. With Python, analytical arguments could be implemented to compare the recorded SWCC of the Clavet sand with each predicted SWCC and asked only to show GSDs that produced a SWCC with $R^2 \geq 0.98$ with the recorded SWCC. Because many calculated GSD parameters sets may only vary slightly from one iteration versus another, the results were filtered further. As a results of the filtering process, three unique solutions were determined for the Clavet sand using this approach.
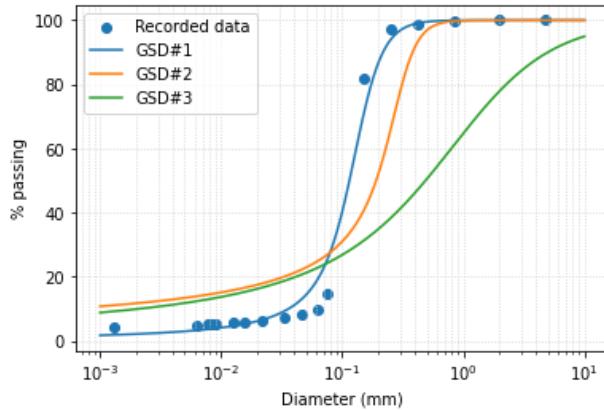
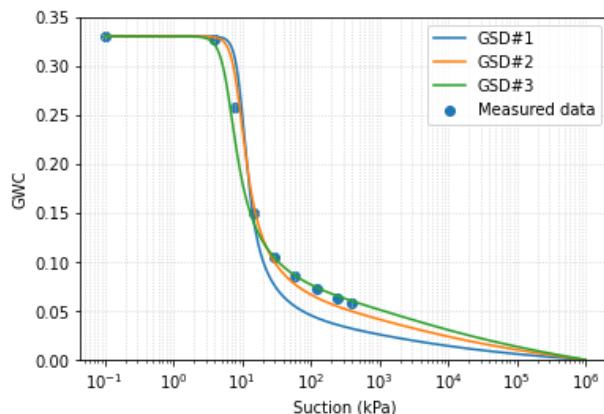Figure 14: Back analyzed GSDs based on Clavet sand properties



Figure 15: Corresponding SWCCs of back analyzed GSDs

Table 3: GSD parameters of back analyzed GSDs

| GSD | $a_{gr}$ | $n_{gr}$ | $m_{gr}$ | $n_p$ |
|------|------|------|------|------|
| #1 | 0.146 | 3.78 | 1.38 | 0.73 |
| #2 | 0.33 | 4.8 | 0.67 | 0.78 |
| #3 | 1.49 | 1.09 | 1.17 | 0.81 |

Table 4: SWCC parameters of back analyzed GSDs

| GSD | $a_f$ | $n_f$ | $m_f$ |
|------|------|------|------|
| #1 | 8.84 | 6.85 | 0.685 |
| #2 | 7.4 | 5.3 | 0.53 |
| #3 | 5.29 | 5 | 0.5 |

From Figure *14*, the first GSD was approximately identical to the measured GSD for the Clavet sand. The second GSD was the determined GSD from the initial analysis, while the final GSD was determined to be a well graded soil when compared to the original soil. As shown in Figure *15*, all three soils were able to produce similar SWCCs when compared to the measured SWCC of the Clavet sand. SWCCs of GSD #1 and #2 had $R^2$ coefficient approximately equal to 0.98, with SWCC of GSD#3 had $R^2$ value of 0.99.

## 7    CONCLUSION

The goal of this research was to construct a method to back analyse a GSD from a given SWCC. The method was achieved by using the Python curve fit function which, utilizes a non – linear least square method. A poorly graded silty sand sample acquired from Clavet was used as the control data to validate the method. The solution provided in Fredlund (2000) was converted into a computational model as a requirement to use the curve fit function. The modified Fredlund method was introduced to overcome numerical and physical limitations determined from Fredlund (2000). A sensitivity analysis of the effect of GSD curve fit parameters and $n_p$ on the prediction of SWCC was also conducted. The following results were made based on the results of this research:

-   The modified Fredlund method was reasonably able to estimate the GSD for the measured SWCC of the Clavet sand.
-   The sensitivity analysis results showed that the variation of grain sizes and grain fractions only seemed to affect the AEV of the soil while the packing structure of the soil heavily influenced the water retention capacity of the soil.
-   The results demonstrate that the back analysis program was successfully constructed to back analyze the recorded GSD of the tested soil. The program was also able to determine different GSDs that produced the same SWCC as the recorded SWCC.

## 8    REFERENCES

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