IMPROVED MATHEMATICAL MODELS FOR PARTICLE-SIZE DISTRIBUTION DATA REPRESENTATION OF TROPICAL WEATHERED RESIDUAL SOILS

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ABSTRACT

There is a need for accurate and cost-effective methods to estimate unsaturated soil property functions. Prior studies have suggested that particle-size distribution data of soils is central and helpful in this regard. This study proposes two improved mathematical models to describe and represent the varied particle-size distribution (PSD) data for tropically weathered residual (TWR) soils. The theoretical analysis and the comparative study of four existing models have indicated that they demand further improvement to handle the PSD of TWR soils. In particular the fixing of curve fitting parameters to the existing models M. Fredlund (2009) [19] result in a wide scatter of the parameters though the impact on the shape of the PSD curve is not significantly visible.

Aiming to improve the existing models, this study, thus proposes unimodal and bimodal models capable of fitting the PSD data of TWR soils more accurately. The new unimodal and bimodal curve fitting models are shown to give an extremely good fit to unimodal and bimodal data. Compared with the other models studied, the new models show a better fit to the soil data analyzed and are highly efficient. The fitting statistics and the range of the optimized parameters are significantly improved. Furthermore, the models developed in this study are of a more general nature and appear to be applicable to a larger range of soil types than those previously published. The newly proposed models greatly simplify and provide reliable PSD data that may be used in physical based prediction of unsaturated soil property functions.

Keywords: Unimodal, Bimodal, Nonlinear Optimization, Curve Fitting

INTRODUCTION

Classical soil mechanics practiced in geotechnical engineering disciplines has confirmed that particle size is a fundamental property of sedimentary materials that tells us much about their origins and history; in particular, the dynamic conditions of transport and deposition of the constituent particles of rocks are usually inferred from their particle size [25]. Size distribution is also an essential property for assessing the likely behavior of granular material under applied fluid gravitational forces, and gauging the economic utility of bulk materials ranging from Gravelly Sands to Silty Clay soil textures [25]. More recently, several researches have pointed out that the grain-size distribution of a soil can form the basis for the prediction of many unsaturated soil properties such as in the prediction of the permeability, compaction and shear strength properties of soils [4,5,7,8,18,21]. A frequent need these days in unsaturated soil mechanics is to fit parameterized models to the PSD data [8]. These include the fitting of adjustable and generalized analytic models to data to predict and correlate with moisture characteristic and hydraulic conductivity curves [4, 7, 8, 20, 21, 23]. The conventional approach of representing the grain size distribution in generating further parameters is cumbersome; and the use of a mathematical function to represent the grain-size distribution provides several benefits to geo-material characterization. This approach has resulted in many simplifications in prediction of unsaturated soil properties [4, 5, 8, 12, 20, and 26]: the soil can be classified using the best-fit parameters; and, the mathematical equation can readily be used as the basis for soil data analysis and description. There is also potential to use the grain-size distribution as a basis for estimating soil behaviors. For example, much emphasis has recently been placed on the estimation of the soil-water characteristic curve (SWCC) using the grain size distribution as a starting point and a mathematical equation can provide a method of representing the entire curve between measured data point [19].

In this regard, many mathematical functions have been suggested for temperate zone soils. However, the PSD of TWR soils display a variety of shapes demanding special attention [26]. In recent developments to fit PSD of different soils using empirical equations, several models have been proposed, such as: Haverkamp-Parlange (1986) [HP – (1986)], Andersson (1990) [AN – (1990)]; the unimodal and the bimodal versions of M. Fredlund (2009) Models [MFU – (2009) and MFB – (2009)].These PSD models along with easily measured soil information such as the density of the soils are commonly used in the Physico-empirical methods to estimate the SWCC [5,6]. Some approaches use the hypothesis of shape similarity between cumulative grain size distribution and the SWCC [9]. In this regard, researchers have provided unimodal and bimodal PSD functions to handle the different nature of the PSD curves to fit well-graded, uniform, and gap-graded soils with different degree of accuracy [20, 21]. However, the numbers of model parameters are relatively large and highly variable. They demand improvement. Moreover, there always remains a need to investigate alternative better models for fitting the PSD of soils.

The SWCC predicted from PSD data can be used to generate and correlate with unsaturated geotechnical properties relatively easily and efficiently and can alleviate the need for the complex and time consuming laboratory procedures required in determining unsaturated soil properties [9, 12, 15]. Numerous investigators have proposed models for the mathematical representation of the PSD of soils mainly for temperate sedimentary/transported soils [4, 7, 8, 15, 18, 21, 26]. However, these models are only capable of addressing certain groups of soils and the fitting performance to the varied nature of the soil matrix greatly depends on the number of parameters used and their simplicity.

In this paper, the objective is to review, evaluate and compare the overall performance of commonly used empirical models and procedures developed for fitting the PSD curve of sedimentary soils and to undertake sensitivity analysis of the fitting performance for the PSD data of TWR soils. From these new modified particle size distribution curve-fitting models usable for unimodal and bimodal PSD data of TWR soils has been developed. This forms, the foundation step for a general procedure to determine the related unsaturated soil property functions.

THEORY, ANALYTICAL PROCEDURES AND DEFINITIONS

To monitor and manage the theory, the analytical procedures and their limitations, the four existing curve fitting models common to geotechnical applications are reviewed and presented first.

Definitions of Important Parameters and Variables

A given soil will be made up of grains of many different sizes and described by the grain size distribution. The main variables are *% Clay, % Silt, % Sand, % of fine* and *% of coarse fractions*. Soil particles are described by the following terms: d = particle diameter (sieve diameter) in mm; $P_p(d)$ = percentage passing of a certain sieve size as a function of particle diameter/size in mm, % Clay = percentage of clay-sized particles present in the soi1 (unified soil classification (USCS) definition is d < 0.005 mm), % Silt = percentage of silt-sized particles present in the soil (USCS definition is 0.005 < d < 0.075mm), % Sand = percentage of Sand-sized particles present in the soi1 (USCS definition is 0.075 < d < 4.75 mm).

Analytical Procedures: Modeling the Particle-Size Distribution Curve

For the past two to three decades, numerous closed-form and empirical equations have been proposed, for common applications in geotechnical engineering, to describe the PSD curve. The analytical procedures used in fitting PSD curves are presented as follows.

M. Fredlund (2009) Unimodal: - MFU – (2009) Model

Eq.(1) is modified from the Fredlund and Xiang (1994) PSD model [11], and is mainly proposed to fit unimodal PSD data[20]. The unimodal fit performs well with the exception of soils exhibiting bimodal appearance. M. Fredlund (2009) unimodal, hereafter MFU – (2009) model [19], has five fitting parameters that have to be optimized as indicated below.

$$P_p(d) = \left\{ \frac{1}{\left\{ \ln\left[\exp(1) + \left(a_{gr}/d \right)^{n_{gr}} \right] \right\}^{m_{gr}}} \right\} \left\{ 1 - \left(\frac{\ln\left(1 + d_{rgr}/d\right)}{\ln\left(1 + d_{rgr}/d_m\right)} \right)^7 \right\} \quad (1)$$

Where: $P_p(d)$ is the % by mass of particles passing a particular size; d is the diameter of any particle size under consideration; a_{gr} is the inflection point on the curve and is related to the initial breaking point on the curve; n_{gr} is related to the steepest slope on the curve (i.e., uniformity of the particle-size distribution); m_{gr} is related to the shape of the curve as it approaches the finer region;d_{rgr} is related to the amount of fines in a soil; d_m is the diameter of the minimum allowable size of particle.

M. Fredlund (2009) Bimodal: - MFB – (2009) Model

Soil texture is sometimes dominated by two or more particle sizes [8, 19]. The MFB – (2009) Model alleviates the problem of using the unimodal model to fit a soil having more than one mode. Nine parameters must be computed when fitting the bimodal equation to PSD data. Seven parameters can be determined using a nonlinear least squares fitting algorithm, and two parameters can be essentially fixed (i.e., d_{rbi} and d_m) [19]. The bimodal version proposed by MF - (2009) [19] is presented in Eq. (2].

$$P_p(d) = \left\{ \left(\frac{w}{\left\{ \ln\left[\exp(1) + \left(a_{bi}/d \right)^{n_{bi}} \right] \right\}^{m_{bi}}} \right) \text{-} \left(\frac{(1-w)}{\left\{ \ln\left[\exp(1) + \left(j_{bi}/d \right)^{k_{bi}} \right] \right\}^{l_{bi}}} \right) \right\} \left[1 - \left(\frac{\ln\left(1 + d_{rgr}/d\right)}{\ln\left(1 + d_{rgr}/d_m\right)} \right)^7 \right] \quad (2)$$

Where: $P_p(d)$ is the % by mass of particles passing a particular size; a_{bi} is related to the initial breaking point along the curve; n_{bi} is related to the steepest slope along the curve; m_{bi} is related to the shape of the curve; j_{bi} is related to the second breaking point of the curve; k_{bi} is related to the second steep slope along the curve; l_{bi} is related to the second shape along the curve; and d_{rbi} is related to the amount of fines in a soil; d is the diameter of any particle size, and d_m the diameter of the minimum allowable size of particle.

Haverkamp-Parlange (1986):- HP – (1986) Model

The HP - (1986) model uses functional forms of PSD curve leading directly to parametric Soil Water Retention functions [16]. The cumulative particle-size distribution function $y_G(x)$ is written in the form given in Eq. (3) as follows:

$$y_G(d) = \left[1 + \left(\frac{D_g}{d} \right) \right]^{-M_s} \quad (3)$$

$$\text{where: } M_s = \left(1 - k_m/N\right)$$

Where: d is the particle size; $D_g$is the particle size scale parameter; $M_s$and$N$are shape parameters of the PSD curve linked to each other in a similar way to the shape parameters used for the SWCC function.

Andersson (1990):- AN – (1990) Model

Andersson (1990) [4] suggests that the *log* mass of the particles is arc - tangent distributed (Cauchy distributed)[4]. Particle size distribution y can be represented using the equation:

$$y = y_o + b \arctan\left[c \log\left(\frac{x}{x_o} \right) \right] \quad (4)$$

Where: x *is* particle diameter, and y_0, b, c and x_0 are parameters. Parameter x_o denotes the most frequent particle diameter corresponding to the cumulative percent y_0. The coordinates x_0 and y_0 correspond to the inflection point; b and c determine the shape of the curve. Parameter c defines how steep the particle-size distribution curve is, i.e. c represents the derivative of the curve at the inflection point.

Arithmetic and Logarithmic PDF

The PSD provides information on the amount and dominant sizes of particles present in a soil and the particle-size probability density function (PDF) is another form that can be used to visualize the distribution of particle sizes [19,21]. The PDF of experimental test data is obtained by differentiating the model fit of the experimental PSD curve. In this regard, to illustrate details of the analysis, the MFU – (2009) model is considered as an example and similar calculations will be performed for other models. The first derivative with respect to "d" is $\mathrm{d}P_p/\mathrm{d}d$, however, plotting $\mathrm{d}P_p/\mathrm{d}d$ in the usual logarithmic plot leads to an arithmetic PDF [19]. As an example, the differentiated form of the MFU – (2009) grain-size model is presented in Eq.(5).

$$\frac{\partial P_p(d)}{\partial d} = [Z_1][Z_2][Z_3] + [Z_4][Z_5] \tag{5}$$

Where:

$$Z_1 = \left\{ \frac{1}{\left(\ln\left[\exp(1) + \left(\frac{a_{gr}}{d} \right)^{n_{gr}} \right] \right)^{m_{gr}}} \right\}$$

$$Z_2 = \left\{ 1 - \left(\frac{\ln\left(1 + \frac{d_{rgr}}{d}\right)}{\ln\left(1 + \frac{d_{rgr}}{d_m}\right)} \right)^7 \right\} \left(m_{gr} \left(\frac{a_{gr}}{d} \right)^{n_{gr}} \right)$$

$$Z_3 = \left\{ \frac{n_{gr}}{d \left\{ \left[\exp(1) + \left(\frac{a_{gr}}{d} \right)^{n_{gr}} \right] \ln\left[\exp(1) + \left(\frac{a_{gr}}{d} \right)^{n_{gr}} \right] \right\}} \right\}$$

$$Z_4 = \left\{ \frac{7}{\left(\ln\left[\exp(1) + \left(\frac{a_{gr}}{d} \right)^{n_{gr}} \right] \right)^{m_{gr}}} \right\}$$

$$Z_5 = \left\{ \frac{\ln\left(1 + \frac{d_{rgr}}{d}\right)^6}{\ln\left(1 + \frac{d_{rgr}}{d_m}\right)^7} \right\} \frac{d_{rgr}}{\left[d^2 \left(1 + \frac{d_{rgr}}{d} \right) \right]}$$

Where: $P_p(d)$is the percentage, by mass, of particles passing a particular size with the diameter of particles in mm; $Z_1, Z_2 \ldots Z_5$ are transformation variables and all other parameters are defined in Eq. (1).

The highest point in the PDF plot is the mode or the most frequent particle size present in the soil mass. Eq. (5) can be arithmetically integrated between the specified particle-diameter sizes. The probability that a particle diameter of the soil will fall in a certain range say, $d_1 < d < d_2$ is determined by the following.

$$\left.\begin{matrix} \text{Probability} \, of \\ (d_1 < d < d_2) \end{matrix}\right\} = \int_{x=d_1}^{x=d_2} P(x) dx \tag{6}$$

The area under the differentiated curve, as expressed in Eq. (7), must equal unity. However, the peak of Eq. (6) will not represent the most frequent particle size because of the logarithmic distribution of the particle-size scale.

$$\int_{x=-\infty}^{x=+\infty} \left(\frac{dP_{\mathrm{p}}}{\mathrm{d}d} \right) dx = 1; \; i.e\!: \mathrm{x} = \text{particle-size di} \tag{7}$$

Therefore, to avoid distortion of the arithmetic PDF function when plotted on a logarithmic scale, it was suggested to represent the PDF function in a manner as shown in Eq. (8) [19].

$$P_1(d) = \frac{dP_p}{\mathrm{d}d} \ln(10) d \qquad [8]$$

Where: $P_1(d)$ is the logarithmic PDF and this is prepared by taking the *log* of particle size and differentiating the grain-size equation, which produces a logarithmic particle size PDF that appears more physically realistic. The peak of Eq. ([8) will represent the most frequent particle size. Therefore, the probability of the logarithmic PDF must be calculated according to Eq. (9).

$$\left.\begin{matrix} \text{Probability} \, of \\ (d_1 < d < d_2) \end{matrix}\right\} = \int_{x=\log(d_1)}^{x=\log(d_2)} p_1(x) dx \qquad [9]$$

The highest point on the Log-PDF plot now is the mode or the most frequent particle size [19,20]. Typical PSD plots for representative groups of soils are indicated in the result and discussions section.

MATERIALS, METHODS AND PROCEDURES

The materials methods and procedures used in testing the existing and the proposed PSD curve fitting models are presented next.

Soil Types, Laboratory Tests and Description of the Data Set analyzed in testing the Models

Grain size distribution tests were conducted with the primary intention of evaluating the applicability of conventional testing procedures to TWR soils. The results indicated that conventional testing procedures could be employed with some modification particularly to sample preparation and testing procedures to take account of the sensitivity of the TWR soils. The details of laboratory tests and the description of the same data set analyzed are explained on some other work by the same authors [2]. Typical PSD curves for several soils were used as the control particle-size test data set on TWR soils and are plotted in Fig. 1.

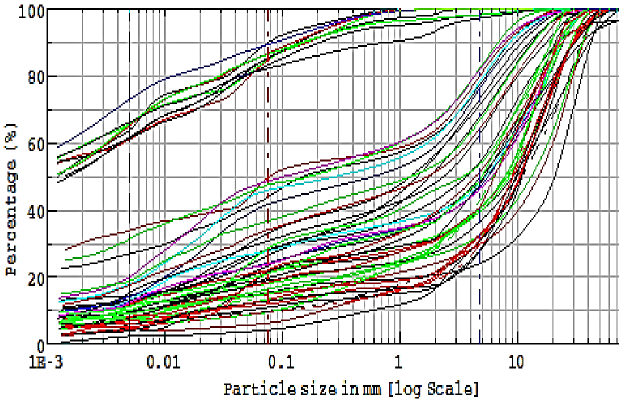


Fig. 1: Particle-size distribution test data on TWR soils used for analysis.

Additional sources of PSD data include: Lyon Associates Institute Inc., (1971); Hailemariam, (1992); Sintayehu, (2003); Abebaw, (2005); Hanna, (2008); Hayimanot, (2008); and Wossen, (2009) etc. [1,3,13,14,17,24,27]. The selected data set provides a wide distribution of soils from a number of different sources, with no bias towards one particular group of investigators. Three types of particle distribution curves namely, well graded, uniform and gap-graded soils are examined.

Curve Fitting Procedures

The MFU - (2009) and MFB - (2009) approaches and the HP - (1986) and AN - (1990) models are used to fit the data. The models are compared and evaluated to select the best fit grain-size distribution model based on the range of the fitting parameters obtained and the concept of whether the models provide a perfect continuous smooth fit of the entire grain-size distribution curve including the coarse and fine extremes or not. Several goodness of fitting statistical measures is used to compare the performance of the models. The mathematical fit of the PSD data provides the basis for developing new procedures and models for predicting a SWCC. As a result, based on the comparative study and analysis of results obtained from the four models, new modified PSD curve-fitting models that best fit the PSD data of TWR unimodal and bimodal soils are proposed and validated. The new models will be compared through a number of statistical goodness of fitting measures with the best of the four published models considered.

Estimation of Model Parameters

The method chosen to estimate parameters depends on whether the model is linear or nonlinear and on the statistical assumptions made concerning measurement errors [8]. Models that are linear (or linearizable) in their parameters are amenable to direct solution. Nonlinear models require an iterative solution, using a search algorithm to determine the minimum of an objective function, and with starting values for the parameters. As all the models are nonlinear, a nonlinear least square algorithm of MatLab-12 software was used.

The best-fit curve parameters were determined using *Levenberg-Marquardt* and *Gauss-Newton* nonlinear curve fitting optimization algorisms of the MatLab-12 software. In this regard, the best curve fitting model parameters and the corresponding goodness of fitting statistics were obtained.

Statistical Methods for Model Validation and Comparisons: Available Methods

Statistical methods are used to validate and compare the curve fitting models against each other. The Sum of Squares due to Error (SSE), the coefficient of multiple determinations (R^2), and the degrees of freedom adjusted *R-Square* (*Adj.* R^2)*;* the Root Mean Squared Error (RMSE) and calculated Akaike Information Criteria (AIC) of the data have been determined for the different models. AIC is used to find which model would best approximate the recorded data. It can simultaneously compare nested or non-nested models. Not relying on the concept of significance, AIC is founded on the maximum likelihood to rank the models. For each model, the AIC value is calculated using:

$$AIC = \begin{cases} when: N/K < 40 \\ N \ln\left(\dfrac{RSS}{N}\right) + 2K \end{cases} \qquad (10$$

$$AIC = \begin{cases} when: N/K \geq 40 &) \\ N\ln\left(\dfrac{RSS}{N}\right) + 2K + \dfrac{2K(K+1)}{(N-K-1)} \end{cases}$$

Where: N is the number of data points, K is the number of parameters plus one, and RSS is residual sum of square of fit.

RESULTS AND DISCUSSIONS

The analysis of the effect of the different parameters used in the curve fitting models and the result of statistical goodness of fit for comparison of the models with various particle-size data are presented.

Comparison of Existing PSD Curve Fitting Models

All PSD data of TWR soil samples were fitted first with the four existing models as the typical plots in Fig. 2.

The precision of results obtained using the nonlinear least squares regression algorithm, which were used to adjust the parameters to fit the model to each PSD data, depends on the initial guesses and the number of iterations. In this regard the corresponding curve fitting parameters and the required goodness of fitting statistics are computed as required with the objective of studying the curve fitting performance of the models to the PSD of TWR soils. The curves fitted to all the experimental PSD data must be smooth and should pass through the measured points.

Typical experimental data from Group - A (BN: P1:1 and BN: P1:2) and from Group - B (NG: P5:1 and NG: P5:2) soil types fitted using the four PSD models representative of different gradation are indicated on Fig. 2.

In all cases, compared to the MFU - (2009) and MFB - (2009) models, the HP - (1986) and AN-(1990) PSD curve fitting models performed least for almost all soils. Compared to the MFU - (2009) model, the MFB - (2009) version has led to a smooth fit passing through all the experimental data points for poorly/relatively gap graded soils. For soils having a unimodal character, both models perform relatively well. The typical plots in Fig. 2 support the above observations.

The use of HP - (1986) and AN - (1990) models performed the least best in all measures of goodness of fitting statistical measures and are not recommended for use in particle size data fitting of TWR soils. As a result, MFU - (2009) and MFB - (2009) models are selected for further study and comparison.

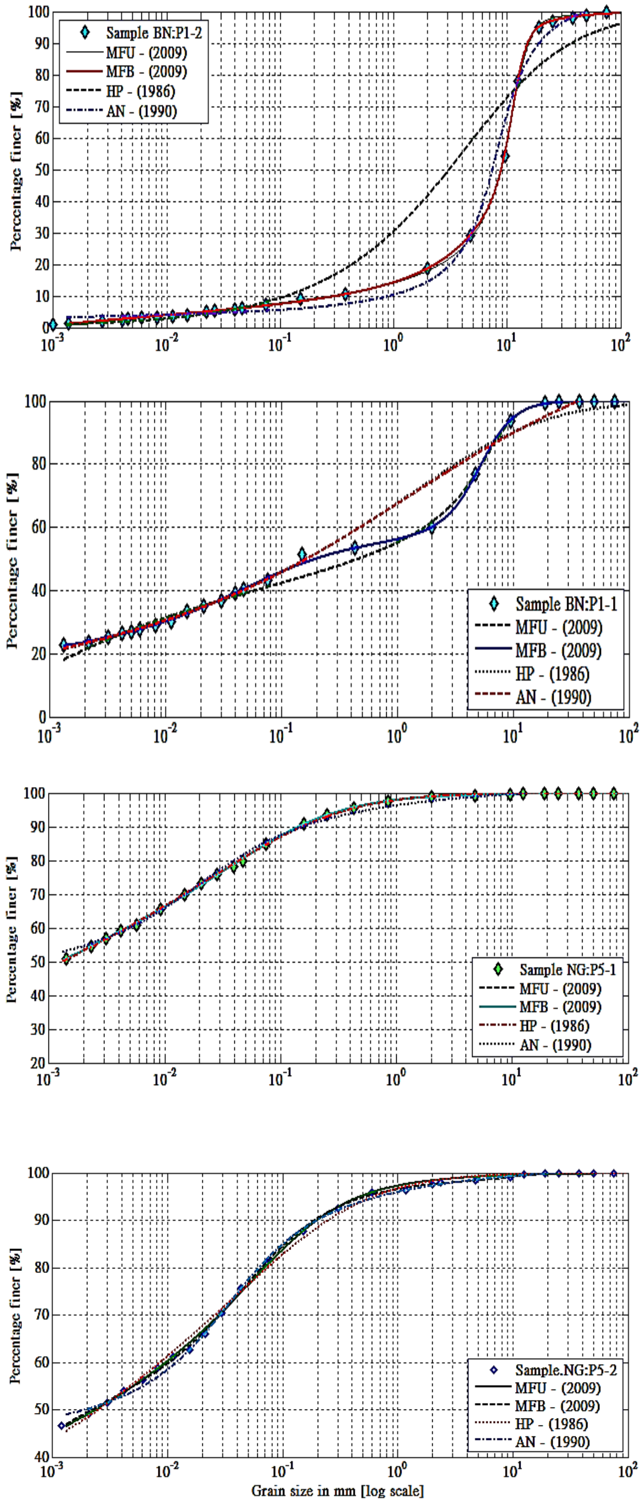


Fig. 2: Typical experimental data fitted using the four PSD models for soils of different gradation

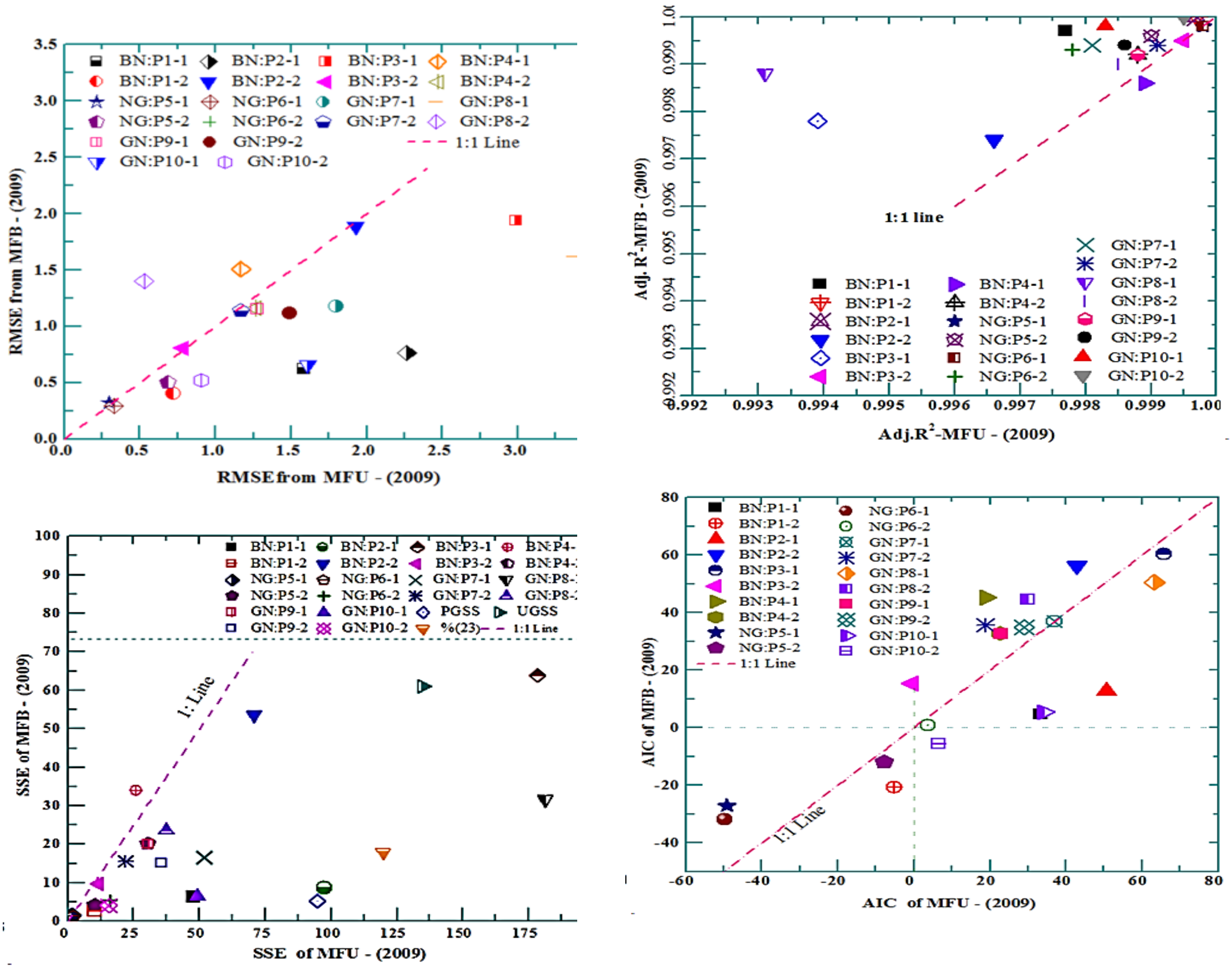


Fig. 3: Statistical Goodness Fit Comparison between Unimodal and Bimodal MF - (2009) Models using Control PSD Data.

With the exception of a few soil samples, comparisons of the SSE, RMSE, Adj. R^2 and AIC values of the two selected PSD models, as shown in Fig. 3 are in favor of the MFB - (2009) model; this suggests that coarser textured TWR soils are bimodal in nature. A smaller SSE, RMSE, AIC and a higher Adj. R^2 (greater than 0.999) were obtained for these soils. These are also in agreement with the PSD nature of TWR soils. The PSD of TWR soils most commonly tend to be poorly graded and may contain more than two dominant sizes in equal proportion.

Typical particle size logarithmic probability density function (Log - PDF) plots with experimental and best fit curves using MFU - (2009) and MFB - (2009) models for TWR soils of (Pit: 1, BN: P1-1) and (Pit 5, NG: P5:1) are shown in Fig. 4, as suggested by Murray, et al., (2000) [20] and Murray, (2009) [19], Log-PDF plots are vital to identify the mode of the PSD curves. Parametric study of the MFU - (2009) and MFB - (2009) models used was undertaken by varying a single parameter keeping the remaining fitting parameter constant. In this regard first, Murray, et al., (2000) [20] and Murray, (2009) [19], studied the meaning of each fitting parameter used in the respective MFU - (2009) and MFB - (2009) curve fitting models [19,20,21]. However, it is noticed that some of the curve fitting parameters such as d_{rgr}, d_{rbi} and d_m display a very wide scatter (range). For example curve-fitting optimization using MFU - (2009) models leads to a minimum d_{rgr} of 5.943 and a maximum d_{rgr} of 13,070,000.

However, this study has shown that fixing these parameters leads to significant change and errors when fitting the finer portion of the curve. Therefore, it is concluded that both MFU - (2009) and MFB - (2009) models either are over parameterized or they demand some modification particularly on the part of the model where

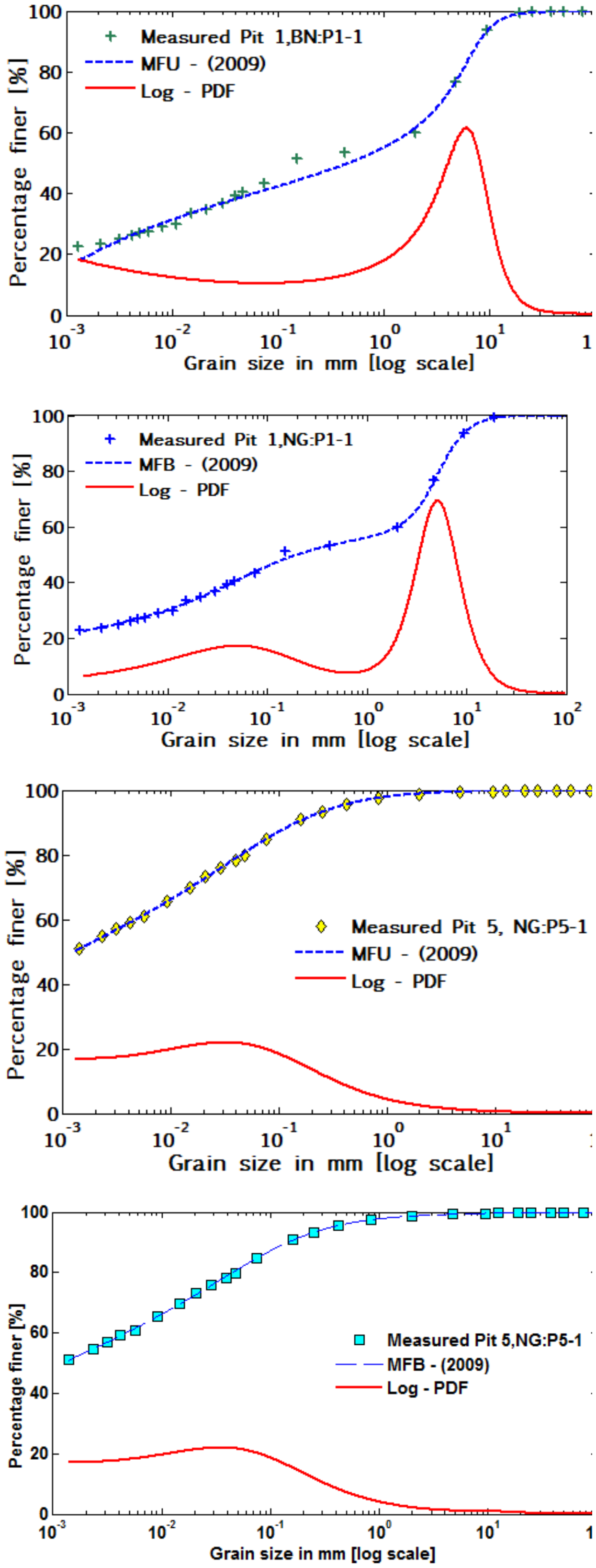


Fig. 4: Typical Particle size Log-PDF plots with experimental and best fit curves using MFU - (2009) and MFB - (2009) models for (Pit: 1, BN: P1-1) and (Pit 5, NG: P5:1).

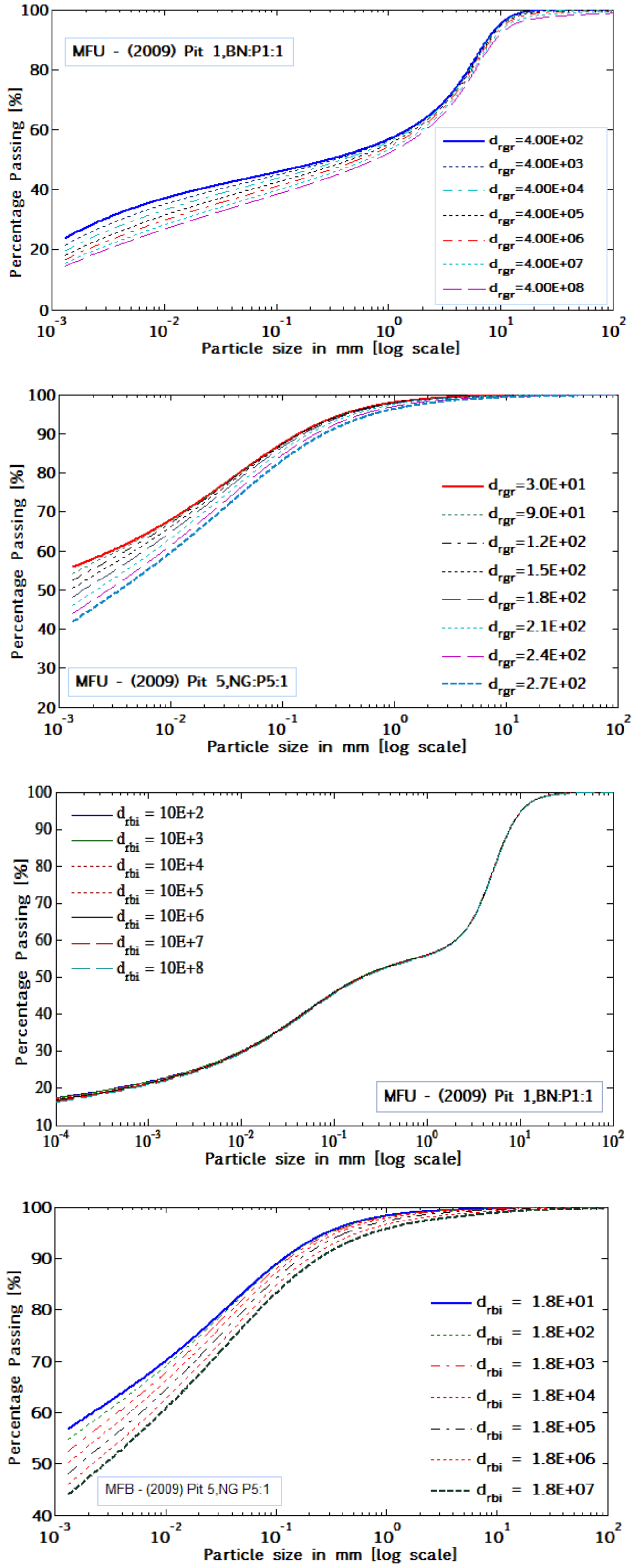


Fig. 5: Effect of varying the d_{rgr} and d_{rbi} parameter for MFU - (2009) and MFB - (2009) fit for (Pit: 1, BN: P1-1) and (Pit 5, NG: P5:1).

d_{rgr}, d_{rbi} and d_m parameters are included. Moreover, during the curve fitting of PSD data, it has been noticed that parameters d_{rgr}, d_{rbi} and d_m are less sensitive to change; as a result, no significant changes on the shape of the fitted curves were displayed for a significant change of these parameters. The sensitivity of d_{rgr} and d_{rbi} curve fitting parameters in the MFU - (2009) and MFB - (2009) model for (Pit: 1, BN: P1-1) and (Pit 5, NG: P5:1) studied are shown in Fig. 5. Murray, et al., (2002) [21] and Murray, (2009) [19], recommended to use 1000 and 0.0001 for d_{rgr} and d_m parameters, respectively.

Proposed Models: Curve Fitting and Determination of Fitting Parameters

With the objective of simplifying and improving the fitting performance of MFU - (2009) and MFB - (2009) models, the study made in this section leads to two improved curve fitting models, namely Model - I and Model - II that best fit the unimodal and the bimodal characteristics respectively of the PSD data of TWR soils.

Assumptions used in the New Models

The number of fitting parameters used in the MFU - (2009) and MFB - (2009) curve-fitting models are the optimum number that lead to neither under-fitting nor over-fitting of the particle size data, as a result the same number of parameters are used in the proposed models, Model-I and Model-II. The two new models proposed narrow the wide scatter in some of the parametric values obtained in both the MFU - (2009) [19] and MFB - (2009) models with new curve fitting parameters.

The coarser and the finer particle-size distribution percentages are dependent on each other, meaning that when the percentage of one size group, say clay, is changed, there will be a direct impact on the percentage amount of other groups such as silt, sand and gravel. The models must account for this behavior. As the goodness of fitting statistical measures used to assess the models MF - (2009) [19] such as R^2, does not adequately express the model's improved performance, other statistical goodness of fitting measures, such as SSE, RMSE and AIC, are used to show the improvements obtained. In this regard, the two newly proposed improved models lead to better statistical goodness of fitting measures. The two new equations provide great flexibility for fitting a wider variety of soils.

Model-I: Proposed Unimodal PSD Curve Fitting Model

An attempt has been made to modify the MFU - (2009) model[19], the unimodal model, to better fit the experimental PSD data of TWR soils. Based on the study of the different particle size curve fitting models previously described, the correction part of the MFU - (2009) model is modified as shown in Eq. (11). The same PSD data of TWR soils used to test the MF - (2009) models [19] have been used to test the new unimodal model.

$$P_p(d)=\left\{\frac{1}{\ln\left[\exp(1)+\left(\frac{\eta}{d}\right)^{\beta}\right]^{\alpha}}\right\}\left\{1-\frac{\chi}{\left[\exp\left(1+\exp\left(\frac{d-\phi}{\phi}\right)^{\eta}\right)^{\beta}\right]^{\alpha}}\right\} \tag{11}$$

Where: $P_p(d)$ is the percentage, by mass, of particles passing a particular size with the diameter of particles in mm; η, β, α, χ and ϕ are Model – I curve-fitting parameters.

Nonlinear curve fitting, determination of fitting parameters and comparison with previous Unimodal PSD Models

Table 2 show some of the statistical values of the optimized curve fitting parameters (η, β, α, χ *and* ϕ) obtained using Model-I and the unimodal and bimodal PSD data respectively. All measures suggest that the curve-fitting parameters are within a narrow range for the unimodal data. The use of Model-I for the bimodal data gives a wider range than for the unimodal data but yields a significantly better fit than the corresponding model proposed by MF - (2009) models [19]. The computed goodness of fitting statistical measures such as SSE, Adj.R^2, RMSE and AIC are plotted against a one-one equality line with the results obtained from corresponding MFU - (2009) model [19], and are shown in **Error! Reference source not found.**. The lower SSE, RMSE, and AIC results obtained suggest, the newly proposed unimodal model (Model-I) is a better fit than the MFU - (2009) model for almost all bimodal data. The R^2 and Adj. R^2

results are almost equal for both unimodal models and do not statistically reflect the improvement in modeling. The SSE and AIC parameters have been found best to compare the models. In this regard, for all the cases considered SSE, RMSE and AIC values are significantly improved, however the unimodality of the particle size data of the Group-B soils make the proposed unimodal model most suitable for these types of soils. Unlike some parameters found in the MFU - (2009) curve-fitting model, the variations of the individual curve fitting parameters do not have large scatter and produce significant improvement by adjusting the shape of the fitted curve.

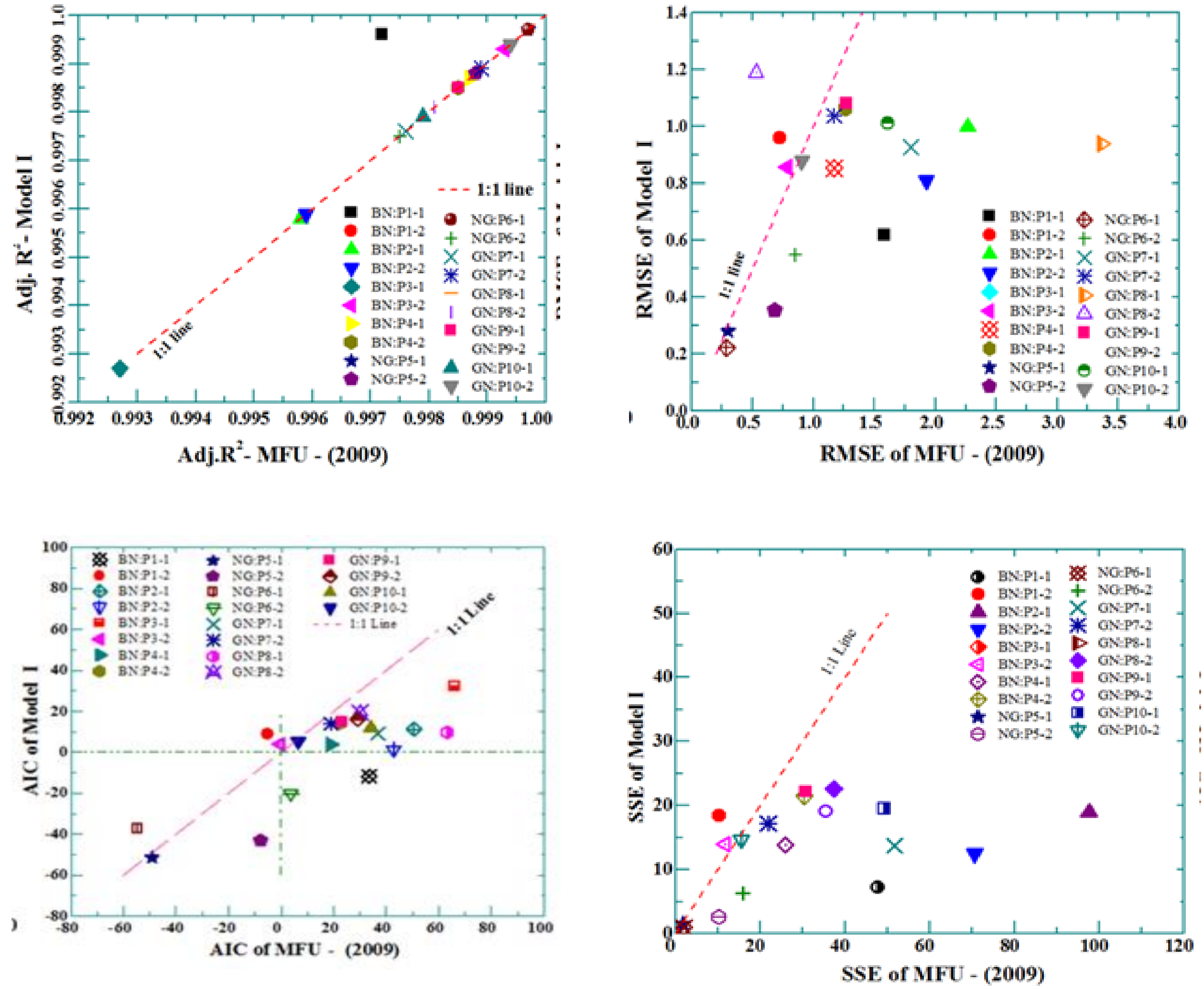


Fig. 6: Statistical Goodness Fit Comparison between Model-I (New unimodal model) and MFU - (2009) models using control PSD data

Table 1.The optimized curve fitting parameters (η, β, α, χ and ϕ) and some statistical measures of using Model-I for unimodal PSD data

Parameter	Mean	Min.	Max.	Range
η	0.1052	0.0529	0.1417	0.0888
β	0.9580	0.7712	1.1010	0.3298
α	0.4826	0.3484	0.6311	0.2827
χ	0.0429	0.0017	0.0654	0.0637
ϕ	0.6768	0.0177	1.0250	1.0073

Table 2.The optimized curve fitting parameters (η, β, α, χ and ϕ) and some statistical measures of using Model-I for bimodal PSD data

Parameter	Mean	Min.	Max.	Range
η	0.2490	0.0025	3.2110	3.2085
β	2.0130	0.5274	7.8250	7.2976
α	1.2010	0.3712	4.8630	4.4918
χ	72.190	1.5900	816.80	815.21
ϕ	1.9950	0.0631	11.430	11.367

The results indicate that the proposed unimodal particle size data-fitting model better fits the unimodal PSD data of TWR soils and can be used effectively whenever discreet and functional textural information is required in the study of unsaturated soil property function predictions.

To display the PSD differently and utilize the additional features of the model, the Particle-Size Log Probability Density Function (PDF) of the experimental test data has been determined using Eq. ((12).

$$\frac{\partial P_p}{\partial d} = [AU_1][1-AU_2][AU_3]+[AU_2][AU \quad (12)$$

Where:

$$AU_1 = \left\{ \frac{1}{\ln\left[exp(1) + \left(\frac{\eta}{d}\right)^{\beta} \right]^{\alpha}} \right\} \alpha \left(\frac{\eta}{d}\right)^{\beta}$$

$$AU_2 = \left\{ \frac{\chi}{\left(exp\left[1 + exp\left(\frac{d-\phi}{\phi} \right)^{\eta} \right]^{\beta} \right)^{\alpha}} \right\}$$

$$AU_3 = \left\{ \frac{\beta}{\left(d\left[exp(1) + \left(\frac{\eta}{d}\right)^{\beta} \right] \ln\left[exp(1) + \left(\frac{\eta}{d}\right)^{\beta} \right] \right)} \right\}$$

$$AU_4 = \left\{ \frac{1}{\ln\left[exp(1) + \left(\frac{\eta}{d}\right)^{\beta} \right]^{\alpha}} \right\} \left\{ \left(\frac{\eta\alpha\beta}{\phi}\right) exp\left(\frac{d-\phi}{\phi}\right)^{\eta} \right\}$$

Where: the parameters presented in the PDF, are the same as the variables defined in Eq. (11) and AU_1, $AU_2 ... AU_4$ are transformation variables.

Typical plots of fit using Model-I with the experimental data and the particle size Log-PDF plots are presented in Fig. 7 and Fig. 8.

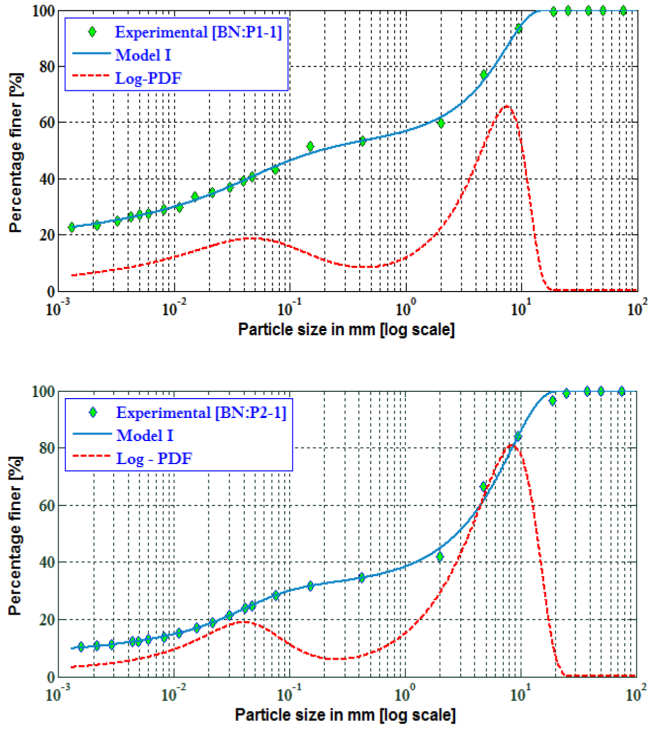


Fig. 7: Typical particle size Log - PDF plots with experimental and best fit curves using Model-I (unimodal model) for various textured soils (Pit: 1, BN: P1-1) and (Pit: 2, BN: P2-1)

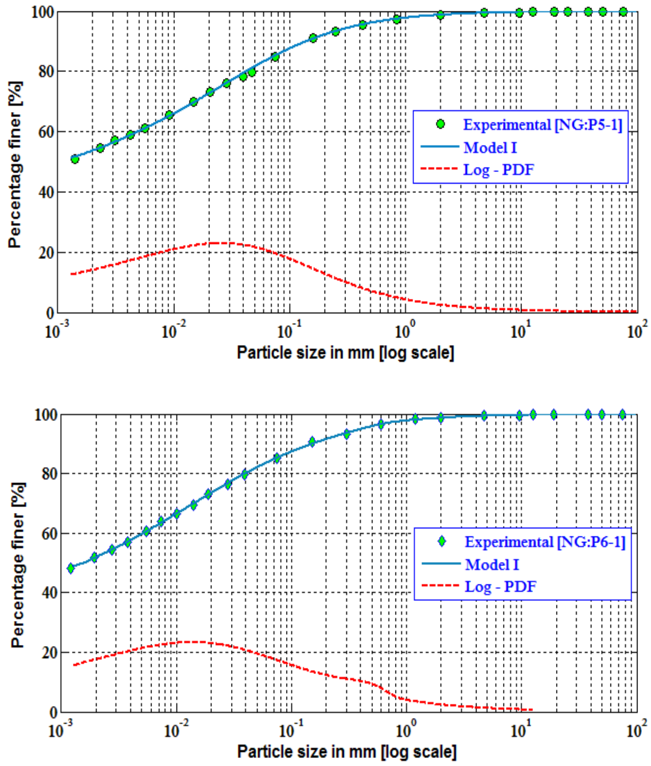


Fig. 8: Typical particle size Log - PDF plots with experimental and best fit curves using Model-I (unimodal model) for various textured soils (Pit 5, NG: P5:1).and (Pit 6, NG: P6:1).

The new proposed unimodal Model - I improve the Log - PDF curve, which clearly points to the position of the mode values. The new proposed model also has the capability of displaying other modes in the range if they exist. The particle size Log-PDF plots suggests the majority of the soils as having a bimodal character.

Study of Fitting Parameters in Model - I

The meaning of each fitting parameter (η, β, α, χ and ϕ) used in the new unimodal curve fitting model is investigated by plotting the variation of one parameter and fixing the others. Typical plots are shown in Fig. 9, Fig.10, and Fig. 11.

In this regard, as shown in Fig. 9, the parameter η has been found to influence the position of the initial breaking point on the curve and clearly determines its position by shifting horizontally and vertically. The parameter η identified clearly the initial breaking point of the curve for unimodal data and provides an indication of the largest particle size in the soil. Parameters η and $1/\eta$, also have a capacity to identify the break point of the curve, respectively, for the finer and the coarser segments of the curve for bimodal data.

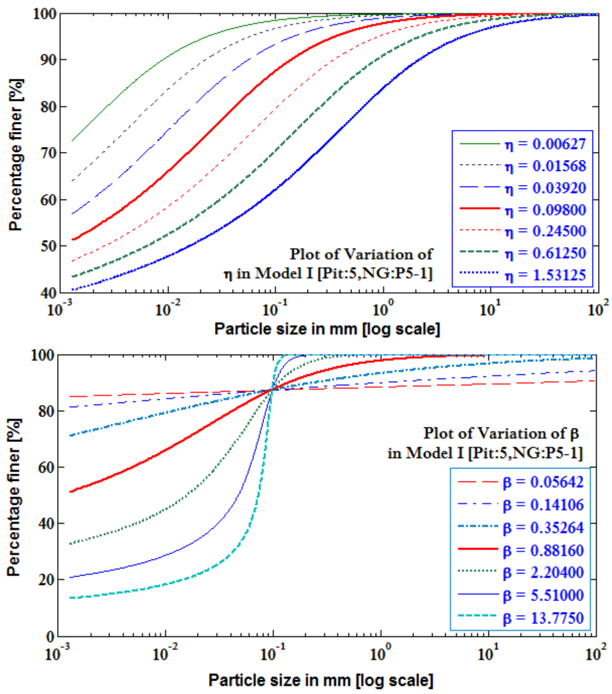


Fig. 9: Effect of varying the η and β parameter for Model-I, unimodal fit for Pit:5, NG: P5-1: $\eta = 0.0981$, $\beta = 0.8749$, $\alpha = 0.4967$, $\chi = 2.524E{-}14$ and $\phi = 0.1448$

The parameter β indicates the steepness of the slope of the middle portion of the curve and significantly affects the grain-size distribution. The larger the β value optimized the steeper the slope. The effect of varying η and β parameters in Model-I, using a typical soil sample from Pit 5 NG: P5-1 is shown in Fig. 9. The effect of varying α and χ parameters in Model-I, using typical soil sample from Pit 5, NG: P5-1 is shown in Fig.10. The parameter α, similar to m_{gr} in the MFU – (2009) model, controls the slope of the initial breaking point of the curve and helps to pinpoint the vertical position of the middle and the finer portion of the curve. Decrease in parameter α shifts the curve vertically up and an increase shifts the curve down. As indicated in Fig. 10, χ is a shape parameter that affects the vertical shift of the whole curve parallel to the first breaking point of the curve and suggests the diameter of the minimum allowable particle size. Its impact depends on the gradation of the soil. Fig. 11 shows that the shape parameter ϕ affects the horizontal shift of the coarser sized portion (upper part) of the curve with a constant slope. This also indicates the initial break of the curve similar to the a_{gr} parameter in the MFU - (2009) model [19].

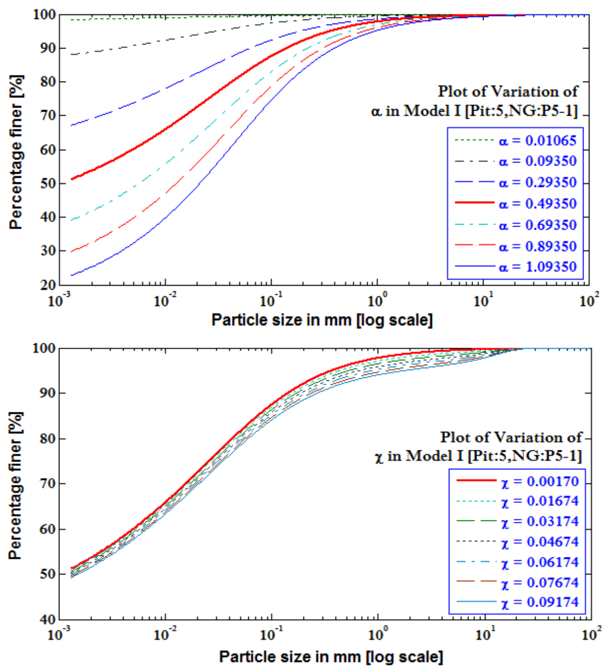
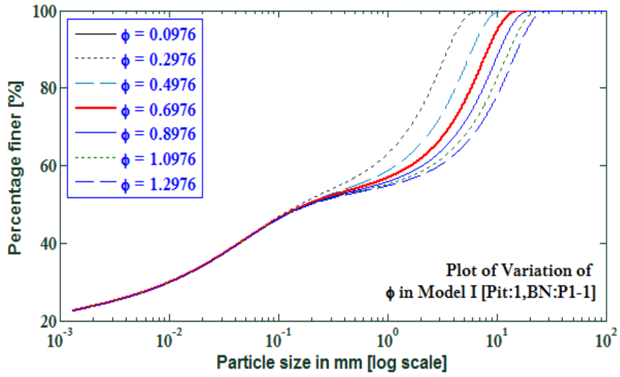


Fig. 10.Effect of varying the α and χ parameter for Model-I, unimodal fit for Pit:5,NG:P5-1: $\eta = 0.0981$, $\beta = 0.8749$, $\alpha = 0.4967$, $\chi = 2.524E{-}14$ and $\phi = 0.1448$.



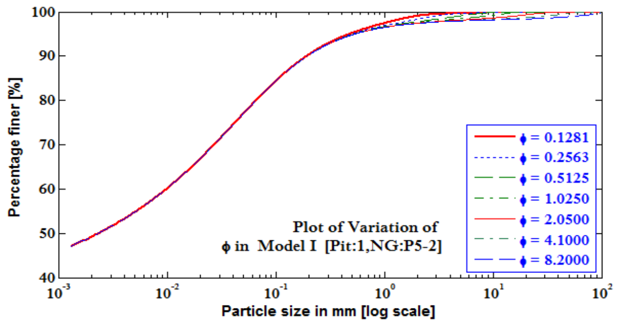


Fig. 11: Effect of varying the ϕ parameter for Model-I, unimodal fit for Pit:1,BN:P1-1: $\eta = 0.1096$, $\chi = 1.59$ and $\phi = 0.6976$ and Pit:5, NG:P5-1: $\eta = 0.098$, $\beta = 0.8749$, $\chi = 2.524E{-}14$ and $\phi = 0.1448$.

Model-II: Proposed Bimodal PSD Curve Fitting Model

From a mathematical standpoint, a gap-graded soil can be viewed as a combination of two or more separate soils. This allows for the "stacking" of more than one unimodal equation [19]. Model - II (new bimodal curve fitting model) is proposed based on the study of the Model-I (unimodal curve-fitting model), and is presented as follows in Eq. (13).

$$P_p(d) = \{\xi[AB_1] + (1-\xi)[AB_2]\}[AB_3] \qquad (13)$$

Where:

$$AB_1 = \left\{ \frac{1}{\ln\left[\exp(1) + \left(\frac{\eta_{bi}}{d}\right)^{\beta_{bi}}\right]^{\alpha_{bi}}} \right\}$$

$$AB_2 = \left\{ \frac{1}{\ln\left[\exp(1) + \left(\frac{\psi_{bi}}{d}\right)^{\lambda_{bi}}\right]^{\theta_{bi}}} \right\}$$

$$AB_3 = \left\{ 1 - \frac{\chi_{bi}}{\left[\exp\left(1 + \exp\left(\frac{d-\phi_{bi}}{\phi_{bi}}\right)^{\eta_{bi}}\right)^{\beta_{bi}}\right]^{\alpha_{bi}}} \right\}$$

Where: $P_p(d)$ is the percentage, by mass, of particles passing a particular size with the diameter of particles in mm; η_{bi}, β_{bi}, α_{bi}, ψ_{bi}, λ_{bi}, χ_{bi} and ϕ_{bi} are Model–II curve fitting parameters; AB_1, AB_2 and AB_3 are transformation variables.

Nonlinear Curve Fitting, determination of fitting parameters and comparison with previous Unimodal PSD Models

The PSD data of TWR soils have been fitted with the new proposed bimodal model (Model-II) Eq. (13). The eight parameters have been optimized against the experimental results.

Table 3 and Table 4 show some of the goodness of fitting statistics of the optimized curve fitting parameters for bimodal and unimodal PSD data, respectively.

All measures suggest that curve-fitting parameters are within a narrow range for bimodal data. The use of Model-II results in a significantly narrower range of fitting parameter than the corresponding range for the MFB – (2009) model. Typical plots using Model - II are shown in Fig. 12.

Table 3. The optimized curve fitting parameters $\eta_{bi}, \beta_{bi}, \alpha_{bi}, \psi_{bi}, \lambda_{bi}, \theta_{bi}$, χ_{bi} and ϕ_{bi} and some statistical measures of using Model-II for Bimodal PSD data

Parameter	Mean	Min.	Max.	Range
η_{bi}	1.771	0.004	9.425	9.421
β_{bi}	3.838	0.894	30.930	30.036
α_{bi}	1.115	0.110	2.932	2.822
ψ_{bi}	3.619	0.000	22.010	22.010
λ_{bi}	2.876	0.554	9.791	9.237
θ_{bi}	239.210	0.422	2670.000	2669.578
χ_{bi}	82.531	0.248	1065.000	1064.753
ϕ_{bi}	10.050	0.091	36.620	36.529

Table 4: The optimized curve fitting parameters $\eta_{bi}, \beta_{bi}, \alpha_{bi}, \psi_{bi}, \lambda_{bi}, \theta_{bi}, \chi_{bi}$ and ϕ_{bi} and some statistical measures of using Model-II for unimodal PSD data

Parameter	Mean	Min.	Max.	Range
η_{bi}	0.063	0.015	0.148	0.133
β_{bi}	2.547	0.771	5.198	4.427
α_{bi}	2.007	0.215	6.267	6.052
ψ_{bi}	0.043	0.006	0.090	0.083
λ_{bi}	1.794	0.660	4.684	4.024
θ_{bi}	3.070	0.070	10.980	10.910
χ_{bi}	1187.3	0.001	3749.0	3748.99
ϕ_{bi}	0.562	0.026	1.669	1.643

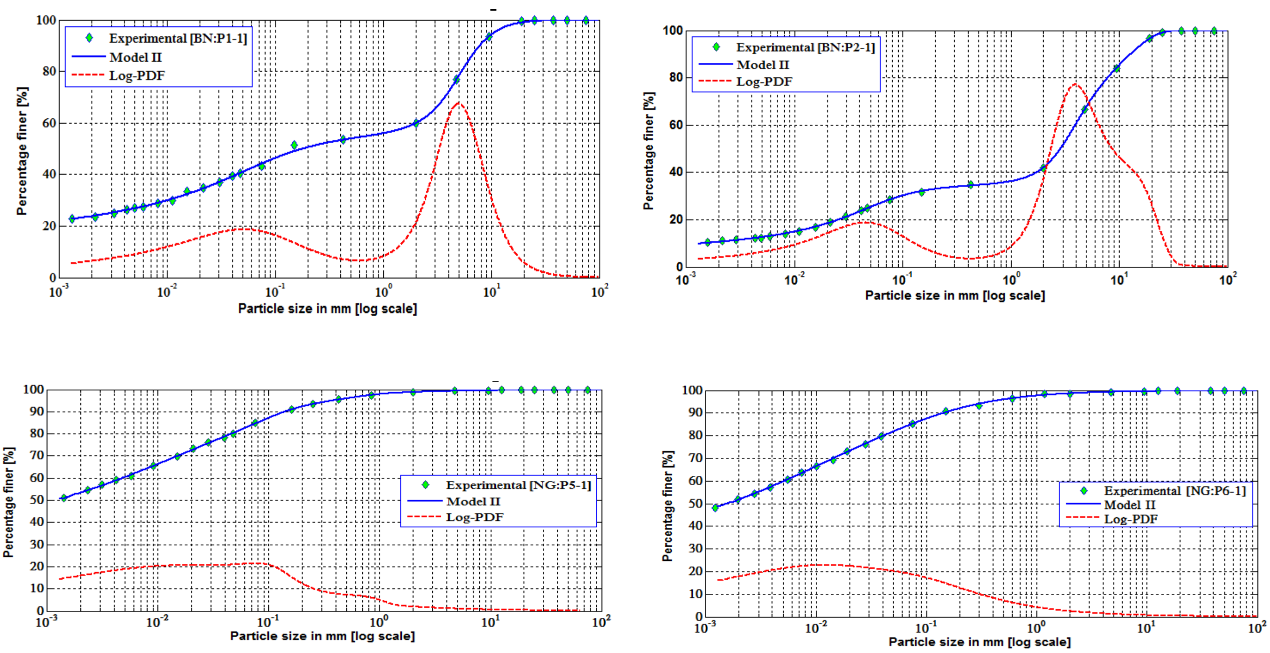


Fig. 12: Typical particle size Log PDF plots with experimental and best-fit curves using Model-II Bimodal fit for representative soil samples

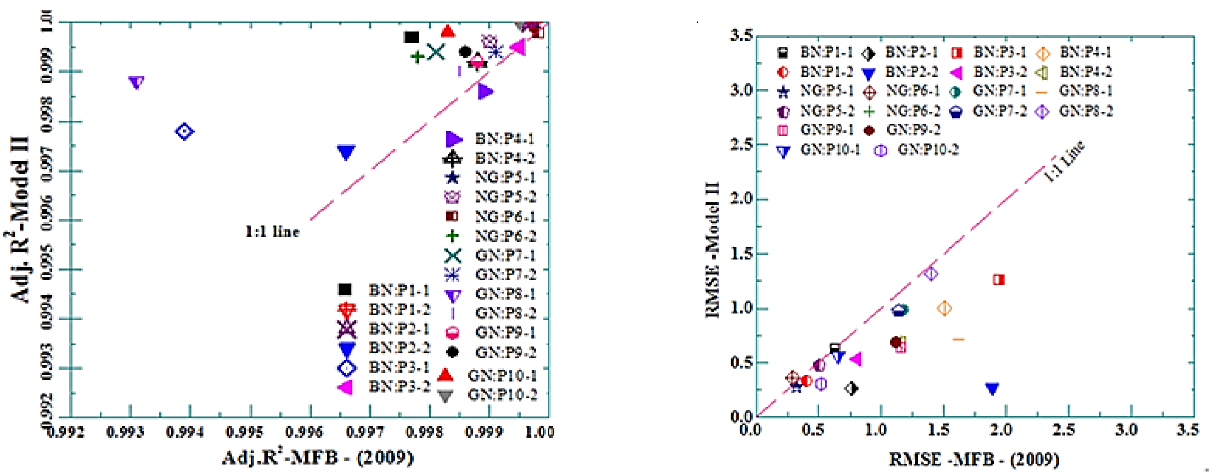


Fig. 13: Statistical Goodness Fit Comparison between Model-II (New Bimodal model) and MFB - (2009) models using control PSD data

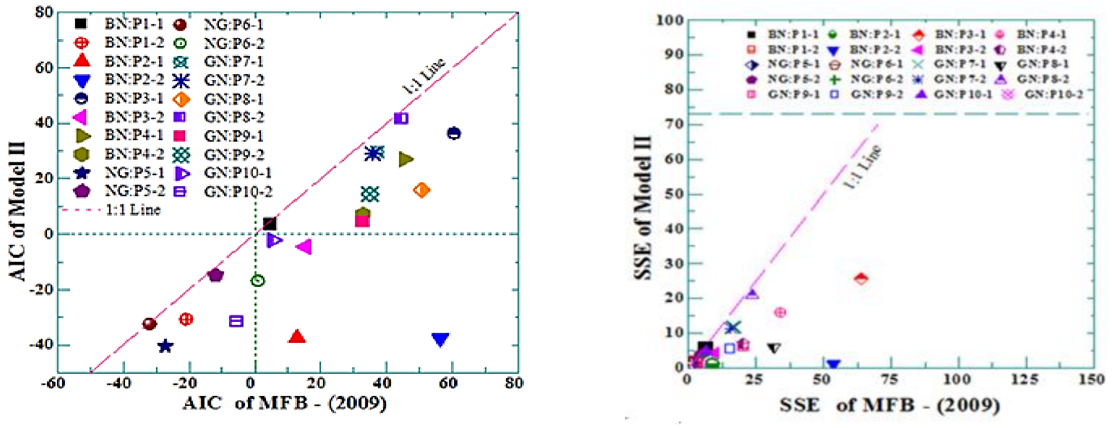


Fig. 14: (Cont…)

The computed goodness of fitting statistical measures such as SSE, Adj. R^2, RMSE and AIC are plotted against a one-one equality line with the results obtained for the corresponding model proposed by MFB - (2009) [*19*] as shown in Fig. 13.

The lower SSE, RMSE and AIC results obtained suggest the proposed bimodal model (Model-II) is an improvement on the MFB - (2009) model for bimodal data and for all unimodal data analyzed. For all the cases considered SSE, RMSE, Adj. R^2 and AIC values are significantly improved and the bimodality of the particle size data of the relatively coarser textured soils make the proposed bimodal model the best for these types of soils. Unlike some parameters found in the MFB - (2009) curve fitting model, the variation of the individual curve fitting parameters does not have a large scatter, and shows significant improvement by adjusting the shape of the fitted curve. The results indicate that the proposed bimodal particle size data-fitting model better fits the bimodal PSD data of TWR soils. Typical plots of fit using the proposed bimodal model and the particle size log-PDF plots are indicated in Fig. 12, Model – II provides significant improvements in the fit of PSD data over previous mathematical representations.

In determination of PDF, the differentiated form of the new bimodal grain-size equation is given as Eq. (14). The double humps in the majority of the PSD data fitted confirm the bimodality of much of the TWR soils as illustrated in Fig. 12.

$$\frac{\partial P_p}{\partial d} = \{[S_1][S_2]+[S_3][S_4]\}[S_5]+[S_6][S_7][\quad (14)$$

Where:

$$S_1 = \left\{ \frac{\xi}{\left[\ln\left[exp(1)+\left(\frac{\eta_{bi}}{d}\right)^{\beta_{bi}}\right]\right]^{\alpha_{bi}}} \alpha_{bi}\left(\frac{\eta_{bi}}{d}\right)^{\beta_{bi}} \right\}$$

$$S_2 = \left\{ \frac{\beta_{bi}}{\left(d\left[exp(1)+\left(\frac{\eta_{bi}}{d}\right)^{\beta_{bi}}\right] \ln\left[exp(1)+\left(\frac{\eta_{bi}}{d}\right)^{\beta_{bi}}\right]\right)} \right\}$$

$$S_3 = \left\{ \frac{1-\xi}{\left[\ln\left[exp(1)+\left(\frac{\psi_{bi}}{d}\right)^{\lambda_{bi}}\right]\right]^{\theta_{bi}}} \theta_{bi}\left(\frac{\psi_{bi}}{d}\right)^{\lambda_{bi}} \right\}$$

$$S_4 = \left\{ \frac{\lambda_{bi}}{\left(d\left[exp(1)+\left(\frac{\psi_{bi}}{d}\right)^{\lambda_{bi}}\right] \ln\left[exp(1)+\left(\frac{\psi_{bi}}{d}\right)^{\lambda_{bi}}\right]\right)} \right\}$$

$$S_5 = \left\{ 1-\frac{\chi_{bi}}{\left(exp\left[1+exp\left(\frac{d-\phi_{bi}}{\phi_{bi}}\right)^{\eta_{bi}}\right]^{\beta_{bi}}\right)^{\alpha_{bi}}} \right\}$$

$$S_6 = \left\{ \frac{\xi}{\left\{ \ln\left[exp(1) + \left(\frac{\eta_{bi}}{d} \right)^{\beta_{bi}} \right] \right\}^{\alpha_{bi}}} + \frac{1-\xi}{\left\{ \ln\left[exp(1) + \left(\frac{\psi_{bi}}{d} \right)^{\lambda_{bi}} \right] \right\}^{\theta_{bi}}} \right\}$$

$$S_7 = \left\{ \frac{\chi_{bi}}{\left(exp\left[1 + exp\left(\frac{d-\phi_{bi}}{\phi_{bi}} \right)^{\eta_{bi}} \right]^{\beta_{bi}} \right)^{\alpha_{bi}}} \right\}$$

$$S_8 = \left\{ \left(\frac{\alpha_{bi}\beta_{bi}\eta_{bi}}{\phi_{bi}} \right) exp\left(\frac{d-\phi_{bi}}{\phi_{bi}} \right)^{\eta_{bi}} \right\}$$

Where: $S_1, S_2 ... S_8$ are transformations variables; the other parameters are the same as the variables used in Eq. (13).

Parametric study of the Model-II: New Bimodal model

A parametric study of the new bimodal equation used has been undertaken by varying a single parameter while keeping the remaining fitting parameter constant. The effect of the following parameters η_{bi}, β_{bi}, α_{bi}, ψ_{bi}, λ_{bi}, θ_{bi}, χ_{bi} and ϕ_{bi} in the fitting of particle size data and their physical meanings are illustrated in Fig. 14.

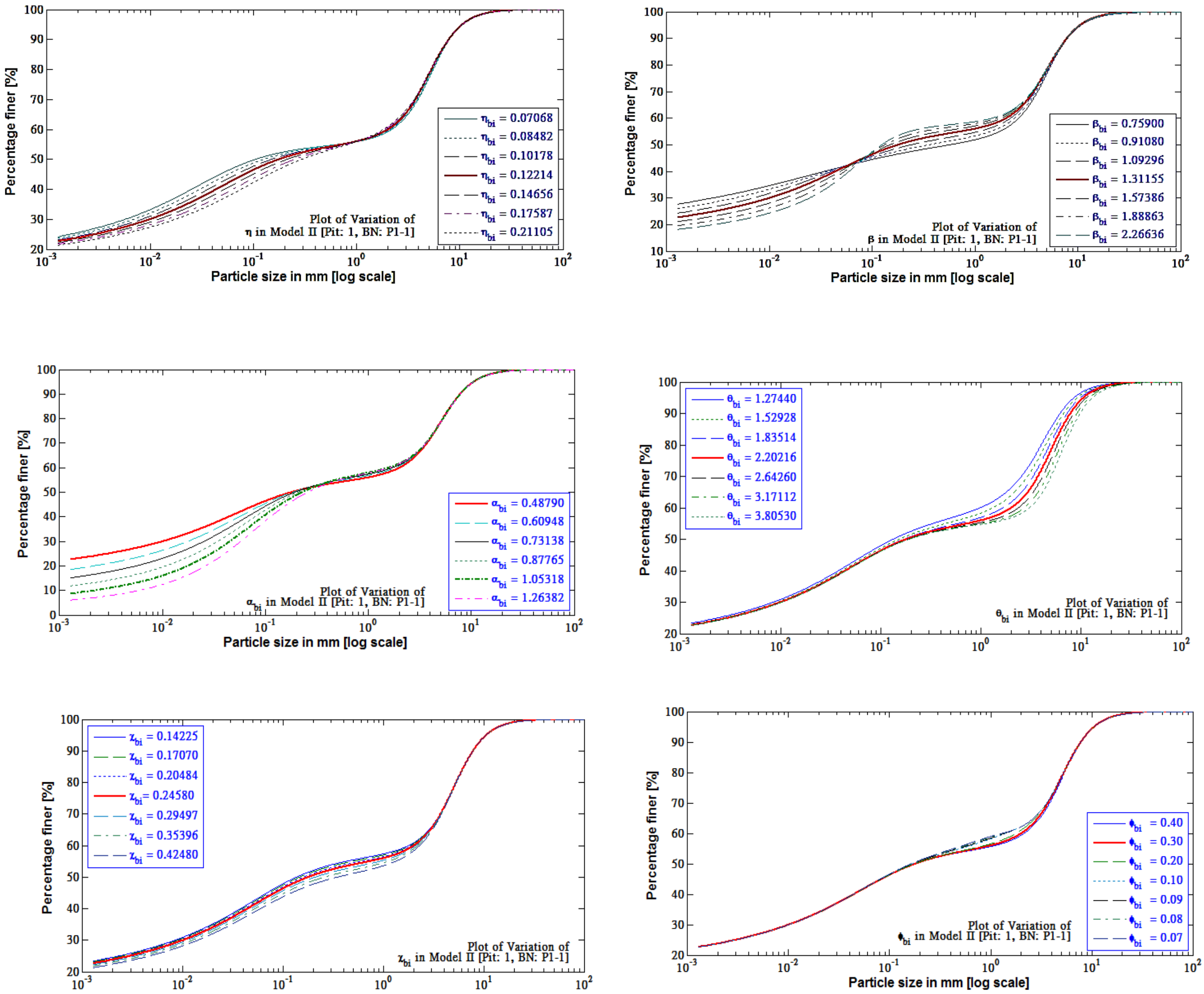


Fig. 15: Effect of varying η_{bi}, β_{bi}, α_{bi}, ψ_{bi}, λ_{bi}, θ_{bi}, χ_{bi} and ϕ_{bi} in Model-II for [Pit:1,BN: P1-1]. While: $\eta_{bi} = 0.12, \beta_{bi} = 1.3$, $\alpha_{bi} = 0.48$, $\psi_{bi} = 5.5$, $\lambda_{bi} = 2.74$, $\theta_{bi} = 2.2$, $\chi_{bi} = 0.25$, $\phi_{bi} = 0.3$, $\xi_{bi} = 0.59$

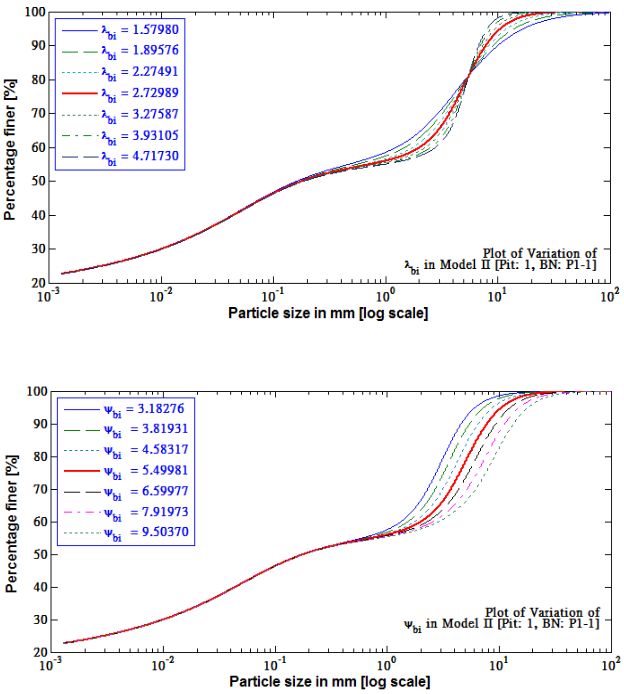


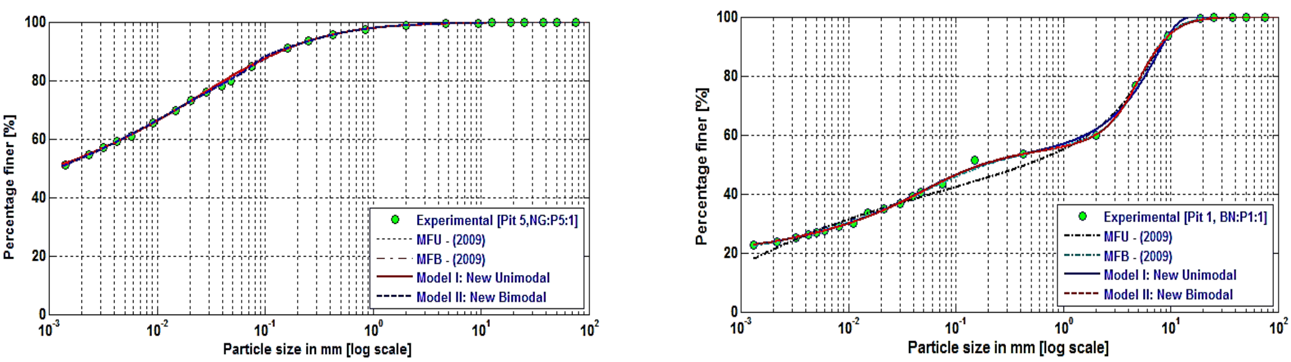
Fig. 16: Cont…

The parameter η_{bi} determines the breaking point towards the finer part of the curve. In this region η_{bi} determines the vertical shift after the breaking point. The β_{bi} parameter determines the slope of the middle and the finer part of the curve at the inflation point and, when β_{bi} increases the shape of the curve becomes flatter. The α_{bi} parameter determines the shape of the last part of the curve and determines the slope of the break point of the curve towards the finer portion. This ψ_{bi} parameter, determines the horizontal shift of the initial break point of the curve towards the middle portion of the curve. This λ_{bi} parameter, determines the slope of the coarser part of the curve at the inflation point; λ_{bi} parameter signifies the vertical rise for a unit horizontal shift in this region. The θ_{bi} parameter determines the flatness of the middle part of the curve.

The χ_{bi} parameter determines the vertical shift of the middle and finer part of the curve. The ϕ_{bi} parameter is a shape parameter which determines the horizontal shift of the break point in the middle portion of the curve. This parameter determines the slope of the middle portion of the curve. All the above parameters are considered better indicators of the curve fit than the MFB - (2009) model.

Comparison of PSD Curve Fitting Models

The new unimodal and bimodal particle size fitting models investigated have been compared with MFU - (2009) and MFB - (2009) models. The four statistical measures of goodness of fit (i.e., SSE, RMSE, R^2, $Adj.\ R^2$ and AIC) are used for comparison purposes. The AIC was found best to illustrate the difference between the models. Data from a typical PSD fitted using the four models are indicated in Fig. 15. These plots and Table 5 support the contention that the two new models lead to smoother and better continuous fits than the MFU - (2009) and MFB - (2009) models.



[a]

[b]

Fig. 17: Comparison of experimental, MFU - (2009), MFB - (2009), Model-I (New unimodal) and Model-II (New bimodal) models fitted totypical:
[a] Group – A TWR soils for Pit 1, BN:P1:1 and
[b] Group – B TWR soils for Pit 5, NG:P5:1.

Table 5. Goodness of fitting statistics and comparison of curve fitting models using AIC.

		Calculated AIC			
Pit No.	Sample	MFU - (2009)	MFB - (2009)	Model - I	Model - II
Pit-1	BN:P1-1	33.497	4.601	-11.791	3.588
	BN:P1-2	-5.260	-20.822	9.058	-30.710
Pit-2	BN:P2-1	50.597	12.767	11.220	-37.150
	BN:P2-2	42.854	56.185	1.266	-37.726
Pit-3	BN:P3-1	65.795	60.403	32.320	36.414
	BN:P3-2	-0.343	15.321	3.937	-4.562
Pit-4	BN:P4-1	18.862	45.275	3.764	27.011
	BN:P4-2	22.622	32.774	14.290	7.180
Pit-5	NG:P5-1	-49.111	-27.187	-51.468	-56.336
	NG:P5-2	-7.780	-11.921	-43.187	-23.404
Pit-6	NG:P6-1	-54.847	-31.918	-37.162	-44.388
	NG:P6-2	3.700	0.882	-20.267	-17.191
Pit-7	GN:P7-1	36.956	37.024	9.122	29.572
	GN:P7-2	18.881	35.677	13.845	29.116
Pit-8	GN:P8-1	63.268	50.555	9.679	15.915
	GN:P8-2	30.137	44.398	19.533	41.839
Pit-9	GN:P9-1	22.975	32.583	15.038	4.447
	GN:P9-2	29.043	34.920	16.019	14.419
Pit-10	GN:P10-1	34.233	5.403	11.909	-2.199
	GN:P10-2	6.541	-5.675	5.176	-31.481
Average AIC		18.131	18.562	0.615	-3.782

Application of Particle Size Distribution Curve Fitting Models

The use of a mathematical model to fit the grain-size distribution provides several advantages in geotechnical engineering [20]. First, models provide a method for estimating a continuous function. Second, soils can be identified based on grain-size distribution by models that are best fit to the data and this information can be stored in a database and used for identification purposes. Third, equations provide a consistent method for determining physical indices such as percent clay, percent sand, percent silt, and particle diameter variables such as d_{10}, d_{20}, d_{30}, d_{50} and d_{60}. The particle size distribution has also been central to several methods of estimating the SWCC. An accurate representation of the soil particle sizes is essential when the grain-size distribution curve is used for such purposes [22].

CONCLUSIONS

The study was undertaken with the primary objective of developing PSD curve-fitting models more suitable for fitting the textural data of TWR soils. In this regard, the performances of four existing particle size data fitting models, namely: the unimodal and bimodal versions of MF - (2009), HP - (1999) and AN - (1990) were first studied. The best PSD curve-fitting model will facilitate the physical based prediction of SWCC from PSD data. The two newly developed PSD curve-fitting models (Model-I and II) were verified using more than sixty PSD test data for TWR soils sampled from western and eastern Ethiopia. Comparisons of the models using the experimentally measured PSD data were assessed based on R^2, Adj. R^2, SSE, RMSE and AIC goodness of fitting statistical measures.

The detailed comparison suggests that MFU - (2009) and MFB - (2009) PSD curve fitting models are better than the HP - (1999) and AN - (1990) methods, which are less accurate. The MFU - (2009) particle size data-fitting model can fit all non-gap graded TWR soils. This was reflected by almost all unimodal particle-size data of Group - B soils of this study. Compared to HP - (1999) and AN - (1990), the MFB - (2009) particle size data-fitting model performed better for all soils, but more suitable and appropriate for gap-graded/bimodal soils. The parametric study on the possibility of fixing some curve fitting parameters, which are indicative of the fitting status of each model, tested against the particle size data of TWR soils, resulted in a wide variability or scatter (range) of the values of parameters. The inconsistent values indicate the fit is determined by a combination of values rather than a single curve fitting parameter. As a result, new unimodal and bimodal particle size data fitting models, Model-I and II respectively have been proposed and validated. The two models have been successfully tested and validated for their applicability for a number of TWR soils and show a marked improvement over the corresponding MF - (2009) models.

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