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Research Article

Keywords: Numerical modelling, Particle distribution, Statistical analysis, Normality test, Minimum sample size

Posted Date: June 9th, 2021

DOI: <https://doi.org/10.21203/rs.3.rs-576711/v1>

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Influence of Particle Distribution on Macroscopic Properties of Particle Flow Model

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Abstract

The particle flow discrete element models for uniaxial compression and tensile tests of rocks are established to study the influence of the particle distribution randomness on the macroscopic mechanical properties of such model. The results of macroscopic mechanical properties show strong discreteness due to the variance of particle distributions, in which compressive strength, tensile strength and Poisson's ratio follow the normal distribution and the Young's modulus follows the negative skewness distribution. The average values of the macroscopic strength obtained based on multiple calculations with different particle distributions should be used for the calibration of microscopic parameters. According to the relationship between sample size and deviation of macro strength averages, the minimum calculation number required to obtain high-precision macro strength with different confidence levels is given.

Key words: Numerical modelling; Particle distribution; Statistical analysis; Normality test;

Minimum sample size

NOTATION

g_1 is the skewness of a statistic

g_2	is the kurtosis of a statistic
U_i	is the i -order center distance of a statistic
$E(X)$	is the expectation of a statistic
$X-E(X)$	is the deviation of a statistic
$Var(X)$	is the variance of a statistic
n	is the size of a statistic
x_j	is the j^{th} order statistic
\bar{x}	is the mean of a statistic
u_i	is the U test coefficient for skewness ($i = 1$) or kurtosis ($i = 2$)
σ_{g_i}	is standard error of skewness ($i = 1$) or kurtosis ($i = 2$)
α	is the specified significance level
$u_{\frac{\alpha}{2}}$	is the U statistic for bilateral tests at the specified significance level
D	is the normal statistic for the LL test
$F^*(X)$	is the cumulative normal distribution function of a statistic
$S_n(X)$	is the cumulative distribution function of a statistic
W	is the normal statistic for the S-W test
x_i	is the i^{th} variable values of a statistic
V	is the covariance matrix of the variable
m_i	is the expected value of i order statistic sampled from the standard normal distribution of the random variable
P	is the significance level corresponding to the statistics when the variable are

tested by LL and S-W

CL is the specified confidence level

μ is the sample mean

δ is the sample variance

n_{min} is the minimum sample size

Z is the value corresponding to the confidence specified in the normal probability distribution table

S is the standard deviation of the population sample

$\Delta_{\bar{x}}$ is the allowable error

1 **1 Introduction**

2 The basic principle of the particle flow discrete element method is to use the collection of
3 particles to simulate the rock and soil, and to duplicate the macroscopic mechanical behavior
4 of such materials through the interaction between particles. It is one of the most popular
5 methods to study the problem of rock and soil mechanics(Hrd *et al.*, 2000; Cook *et al.*, 2004;
6 Onate *et al.*, 2004; McDowell *et al.*, 2006; Qin *et al.*, 2013; Zhang *et al.*, 2015; Zhao *et al.*,
7 2019; Xie *et al.*, 2020). The microscopic parameters of particle flow models are usually not
8 directly equal to the macroscopic mechanical parameters of materials. Simulations of strength
9 tests (uniaxial, biaxial, Brazilian splitting experiments, etc.) are needed to establish the
10 relationship between model microcosmic parameters and the macroscopic mechanical
11 properties of rocks, such a process is called calibration (Xia *et al.*, 2018; Shi *et al.*, 2019). The
12 particle distribution may have a significant influence on the macroscopic mechanical properties
13 of the model because the change of particle locations will affect the crack initiation and
14 propagation in the rock model. Therefore, a one-time simulation under a given particle
15 distribution may not be able to obtain the accurate relationship between microscopic
16 parameters and macroscopic strength in calibrations. This paper studies the influence of the
17 randomness of particle distribution on the macroscopic mechanical parameters of the discrete
18 element model, to improve the calibration accuracy of the particle flow discrete element model.

19
20 Scholars have studied the factors that affect the macroscopic properties. Potyondy *et al.*
21 (Potyondy *et al.*, 2004) found that Young's modulus and tensile strength are strongly correlated

22 with particle size. Yoon, Wang, Castro-Filgueira, Boutt and Martin et al. (Boutt *et al.*, 2002;
23 Cho *et al.*, 2007; Yoon *et al.*, 2007; Wang *et al.*, 2010; Castro-Filgueira *et al.*, 2017) pointed
24 out that the effective stiffness and stiffness ratio of intergranular contact have the greatest effect
25 on Young's modulus, and the relationship between effective contact modulus and Young's
26 modulus is linear. Tangential and normal contact strength have the greatest influence on
27 compressive strength and tensile strength, and the relationship between contact strength and
28 compressive strength is linear. The stiffness ratio has the greatest influence on Poisson's ratio,
29 but only has minor influence on other macro parameters. The particle friction coefficient
30 merely affects the post-peak response of the particle flow model. Wang and Martin et al. (Wang,
31 1981); Schöpfer *et al.*, 2009) found that Young's modulus, uniaxial compressive strength (UCS),
32 tensile strength (T), strength ratio (UCS/T) and internal friction angle would all decrease with
33 the increase of porosity, while porosity had almost no influence on Poisson's ratio. Castro-
34 Filgueira et al. (Castro-Filgueira *et al.*, 2016) studied confining pressure and found that Young's
35 modulus, compressive strength and tensile strength all increased with the increase of confining
36 pressure, but had little impact on Poisson's ratio. Coetzee et al. (Coetzee *et al.*, 2009) showed
37 that the internal friction angle increased with the increase of particle stiffness and friction
38 coefficient, while the friction coefficient had little influence on the system stiffness.

39

40 The above researches have made a lot of achievements in the aspects of model calibration.
41 However, there are still some unsolved problems. The heterogeneity and randomness of natural
42 rocks lead to a significant discreteness of macroscopic mechanical parameters of such material

43 (Yamaguchi, 1970; Ruffolo *et al*, 2009; Cui *et al.*, 2017). For the discrete element model, the
44 randomly distributed particles could be used to simulate the heterogeneous characteristic of
45 rocks, but how does particle distribution affect the macroscopic strength of the model has not
46 been systematically studied yet. In addition, the particle distributions are usually different in
47 the model for calibration and that for solving practical problems. The difference of particle
48 distributions changes the crack initiation location and propagation path, which may have a
49 significant influence on the macroscopic mechanical properties of the model. That is, due to
50 the randomness of particle distribution, two models with the identical microscopic parameters
51 may not provide the same macroscopic strength. The calibration according to only one
52 calculation without the consideration of particle distribution may not correctly reveal the
53 relation between microscopic parameters and macroscopic strength. Therefore, it is necessary
54 to study the coupling effect of the particle distribution and microscopic parameters on the
55 macroscopic strength of the model, and then to propose a statistic-based calibration principle
56 using the average values from multiple calculations.

57

58 In this paper, the particle flow discrete element models for simulating uniaxial
59 compression and tensile tests of rocks are established. Based on a large number of numerical
60 simulations, the relationship between the particle distribution randomness and the macroscopic
61 mechanical response of the model is obtained by using statistical analysis methods. And the
62 minimum sample size required to provide high-precision averages of macroscopic mechanical
63 properties are obtained. The applicability of the "three in five tests for the mean" method

64 (calculate five times with different particle distribution, and obtain the average value after
65 removing the maximum and minimum) for calibration is verified.

66

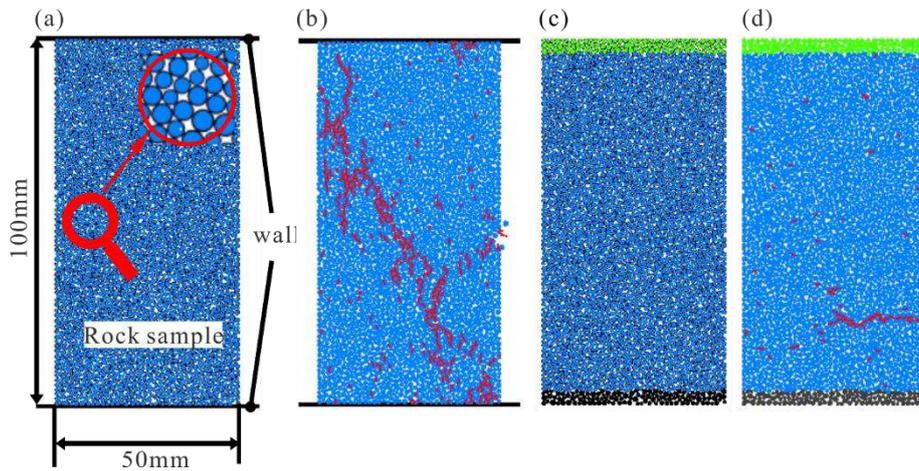
67 **2 Modeling of uniaxial tests for rocks**

68 Natural rocks are characterized by discontinuity, anisotropy, heterogeneity, inelasticity
69 and other inherent characteristics (Jing, 2003). Therefore, for rock modeling the continuum
70 hypothesis may no longer applicable. The particle flow discrete element method is a novel
71 discontinuous medium method, which uses a series of discrete disk (2D) or spherical (3D)
72 particles to model the rock, and to reflects the deformation and failure of rock by the relative
73 position, motion state and bond relationship of the particles. Particle flow discrete element
74 method has unique advantages in simulating large deformation and brittle failure of rocks under
75 various external forces (Mehranpour *et al.*, 2017; Castro-Filgueira *et al.*, 2020; Tian *et al.*, 2020)

76 The Idaho basalt reported in the reference (Moon *et al.*, 2012) is selected as the representative
77 of rocks in this paper. The macroscopic properties of Idaho basalt are: Young's modulus 9.66
78 GPa, Poisson's ratio 0.21, compressive strength 28.4 MPa, and tensile strength 6.6 MPa. The
79 two-dimensional simulations of uniaxial compression and uniaxial tensile tests are used for the
80 calibration, as shown in Fig. 1 (a) and (c). The height and width of the models are 100 mm and
81 50 mm, respectively. Rigid walls are located on the upper and lower sides of the sample for
82 axial loading. The crack distributions inside the rock samples under uniaxial compression and
83 uniaxial tensile load are shown in Fig. 1 (b) and (d), respectively. The microscopic parameters
84 are calibrated according to the traditional method (Castro-Filgueira *et al.*, 2017) without

85 changing particle distribution yet, to obtained the benchmark for the subsequent study. The
 86 macroscopic mechanical properties of the model after calibration are shown in Table 1 and the
 87 corresponding microscopic parameters are shown in Table 2.

88



89

90 Fig. 1 Particle flow models for simulating uniaxial tests and typical results: (a) model for uniaxial
 91 compression tests; (b) crack distribution after uniaxial compression tests; (c) model for uniaxial tensile
 92 tests; (d) crack distribution after uniaxial tensile tests

93

94 Table 1 Macroscopic mechanical properties of particle flow model after calibration

Items	Values		
	Model	Experiment (Moon and Oh, 2012)	Deviation
Young's modulus	9.5 GPa	9.66 GPa	1.66%
Compressive strength	28.63 MPa	28.4 MPa	0.81%
Tensile strength	6.49 MPa	6.6 MPa	1.67%
Poisson's ratio	0.211	0.21	0.48%

95

96 Table 2 Micromechanical parameters of particle flow model after calibration

Categories	Items	Symbols	Values
General	Lower limit of particle diameter, mm	cm_Dlo	2

	Upper limit of particle diameter, mm	cm_Dup	1.66
	Particle density, kg/m ³	cm_densityVal	2650
	Damping coefficient	cm_localDampFac	0.7
Linear contact	Effective modulus, GPa	pbm_emod	6.28
	Friction coefficient	pbm_fric	0.50
	Stiffness ratio	pbm_krat	1.45
Parallel bond	Initial gap tolerance, mm	pbm_igap	0.1
	Radius multiplier	pbm_rmul	1.00
	Effective modulus, GPa	pbm_bemod	6.28
	Stiffness ratio	pbm_bkrat	1.45
	Moment contribution factor	pbm_mcf	1.00
	Average of tensile strength, MPa	pbm_ten_m	16.5
	Standard deviation of tensile strength, MPa	pbm_ten_sd	4.125
	Average of cohesion, MPa	pbm_coh_m	16
	Standard deviation of cohesion, MPa	pbm_coh_sd	4
	Frictional angle, degree	pbm_fa	30.00

97

98 To illustrate the influence of particle distributions on the macroscopic mechanical
99 parameters of the model, ten simulations of uniaxial compression and tensile tests with different
100 particle distributions (all other parameters maintain constant) are performed and the
101 corresponding stress-strain curves are shown in Fig. 2. The results show significant
102 discreteness, where the maximum difference of the simulated compressive strength is over 10
103 MPa, accounting for 30% of the experimental measured value. The tensile strength is also
104 strongly affected by the randomness of particle distributions; the maximum difference of
105 simulated tensile strength in Fig. 2(b) is more than 4.5 MPa, accounting for about 70% of the
106 experimental measured value. The above-mentioned results illustrate the necessity of a
107 systematically investigation on the statistical rule of the particle distribution effect on the
108 macroscopic mechanical properties of the particle flow discrete element model.

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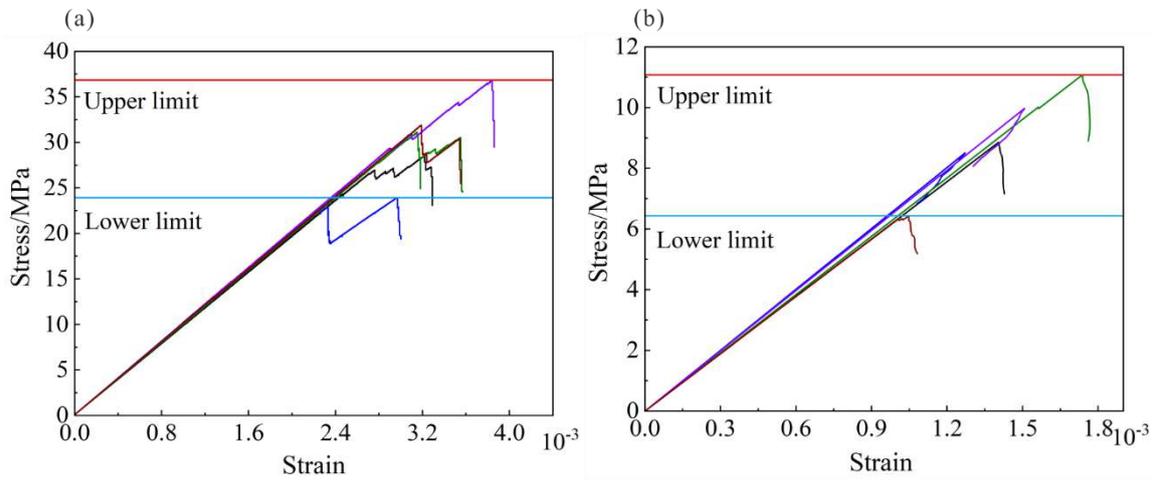


Fig. 2 Stress-strain response: (a) uniaxial compression tests; (b) uniaxial tensile tests

3 Statistical analysis on the results of macroscopic mechanical properties

The results of 500 simulations of rock compression and tensile tests with different particle distribution are collected as the sample base for the following statistical analysis: 1) Conducting normality test to obtain the probability distributions of the simulation results. 2) Determining the minimum sample size that could produce high-precision average values of macroscopic mechanical properties. 3) Examining the precision of average values obtained from the commonly used "three in five tests for the mean" method to verify the applicability of such method in the calibration of particle flow model.

3.1 Normality test

The normality test is commonly used to determine whether a sample follows the normal distribution. The popular normality test methods including skewness and kurtosis coefficient test (U test), Lilliefors test (LL), Shapiro-Wilk test (S-W) and Kolmogorov-Smirnov test (K-S), as well as graphic methods such as Q-Q graph, P-P graph and histogram (Keskin *et al.*,

127 2006; Mohd *et al.*, 2011; Yap *et al.*, 2011; Lee *et al.*, 2016).The applicable scope of the above-
128 mentioned normality test methods has not been clearly defined at present. Taking the S-W
129 method as an example, the references (Mohd *et al.*, 2011) point out that the S-W test is
130 applicable to the case with a sample size greater than 100, while the researcher (Society,R.S,
131 2019) insists that the S-W test is suitable for data with a sample size of 3~2000, and there are
132 also literatures believe that the S-W test is the most accurate approach for any sample size
133 (Mohd *et al.*, 2011; Society,R.S, 2019). Therefore, to ensure the correctness of normal test
134 results, this work comprehensively uses a variety of normality test methods, including the U
135 test, LL test and S-W test, and supplemented by histogram and Q-Q graph.

136

137 The parameters required for the normality tests are shown below.

138 1) Skewness and kurtosis coefficient test

139 Skewness is a parameter that reflects the degree and direction of data distribution skewed,
140 which is defined as (Keskin, 2006; (Trust, 2016):

141
$$g_1 = \frac{\nu_3}{\nu_2^{3/2}} = \frac{E[X - E(X)]^3}{[Var(X)]^{3/2}}$$

142 1.

143
$$\nu_i = \frac{1}{n-1} \sum_{j=1}^n (x_j - \bar{x})^i$$

144 2.

145

146 Kurtosis is a parameter that represents the peak value of the probability density

147 distribution curve at the mean, which is defined as (Keskin, 2006; Trust, 2016):

148
$$g_2 = \frac{\nu_4}{\nu_2^2} - 3 = \frac{E[X - E(X)]^4}{[Var(X)]^2} - 3$$

149 3.

150

151 The corresponding U test value is calculated as:

152
$$u_i = \frac{g_i}{\sigma_{g_i}} (i = 1, 2)$$

153 4.

154

155 The variable rejects the normal distribution hypothesis when $|u_i| > u_{\frac{\alpha}{2}}$.

156

157 2) LL test

158 The key parameter D of LL test is defined as (Yap *et al*, 2011; Mohd *et al*, 2011):

159
$$D = \max |F^*(X) - S_n(X)|$$

160 5.

161

162 When $D > D(n, \alpha)$ (Massey, 1951) ($D(n, \alpha)$ is the statistical threshold of LL test at the
163 specified significance level α and sample size n ; for the same sample size, it decreases with
164 increasing confidence level) the variable rejects the normal distribution hypothesis.

165

166 3) S-W test

167 The S-W test is the first normal test method that can be used to detect deviations in
 168 skewness, kurtosis, or both exist deviation. The key parameters of S-W test is defined as
 169 (Shapiro and Wilk, 1965, 1972; Keskin, 2006; Öztuna, Elhan and Tüccar, 2006; Mohd Razali
 170 and Bee Wah, 2011; Yap and Sim, 2011):

$$171 \quad W = \frac{\left(\sum_{i=1}^n a_i x_i \right)^2}{\sum_{i=1}^n (x_i - \bar{x})^2}$$

172 6.

$$173 \quad a_i = (a_1, \dots, a_n) = \frac{m^T V^{-1}}{\sqrt{(m^T V^{-1} V^{-1} m)}}$$

174 7.

$$175 \quad m = (m_1, \dots, m_n)^T$$

176 8.

177

178 When $W < W(n, \alpha)$ ($W(n, \alpha)$ is the statistical threshold of S-W test at the specified
 179 significance level α and sample size n , it increases with significance level for the same sample
 180 size) the variable X rejects the normal distribution hypothesis.

181

182 The above-mentioned methods are applied to implement the normality tests for the
 183 simulated macroscopic property results of rock models with different particle distributions. The
 184 confidence coefficient is set to be 95% (i.e. confidence level $CL=0.95$, significance level
 185 $\alpha=0.05$), and the results of normality test are shown in Table 3. The skewness U test value u_1

186 of the Young's modulus is -4.45, which are without the range of -1.96~1.96 ($\alpha=0.05$ look-up
 187 the normal distribution table has $u_{\frac{\alpha}{2}}=1.96$); and the significance level P (P is the significance
 188 level corresponding to the statistics when the variable are tested by LL and S-W) of both the
 189 LL test and the S-W test is 0.015 and 0, respectively, which is less than the corresponding
 190 confidence standard $\alpha=0.05$. It can be seen from Fig. 3 (a) and Fig. 4 (a) that the frequency
 191 distribution histogram is in poor agreement with the normal distribution curve, a large number
 192 of data points are outside the standard range corresponding to the confidence level of the Q-Q
 193 graph. To sum up, Young's modulus do not obey normal distribution.

194

195 According to Table 3, Fig. 3 and Fig. 4, all normal test statistics of compressive strength,
 196 tensile strength and Poisson's ratio are within the standard range corresponding to the
 197 confidence level. And the frequency distribution histogram is in good agreement with the
 198 normal distribution curve, and few data points in the Q-Q diagram are beyond the standard
 199 range of confidence levels. In conclusion, compressive strength, tensile strength and Poisson's
 200 ratio obey normal distribution.

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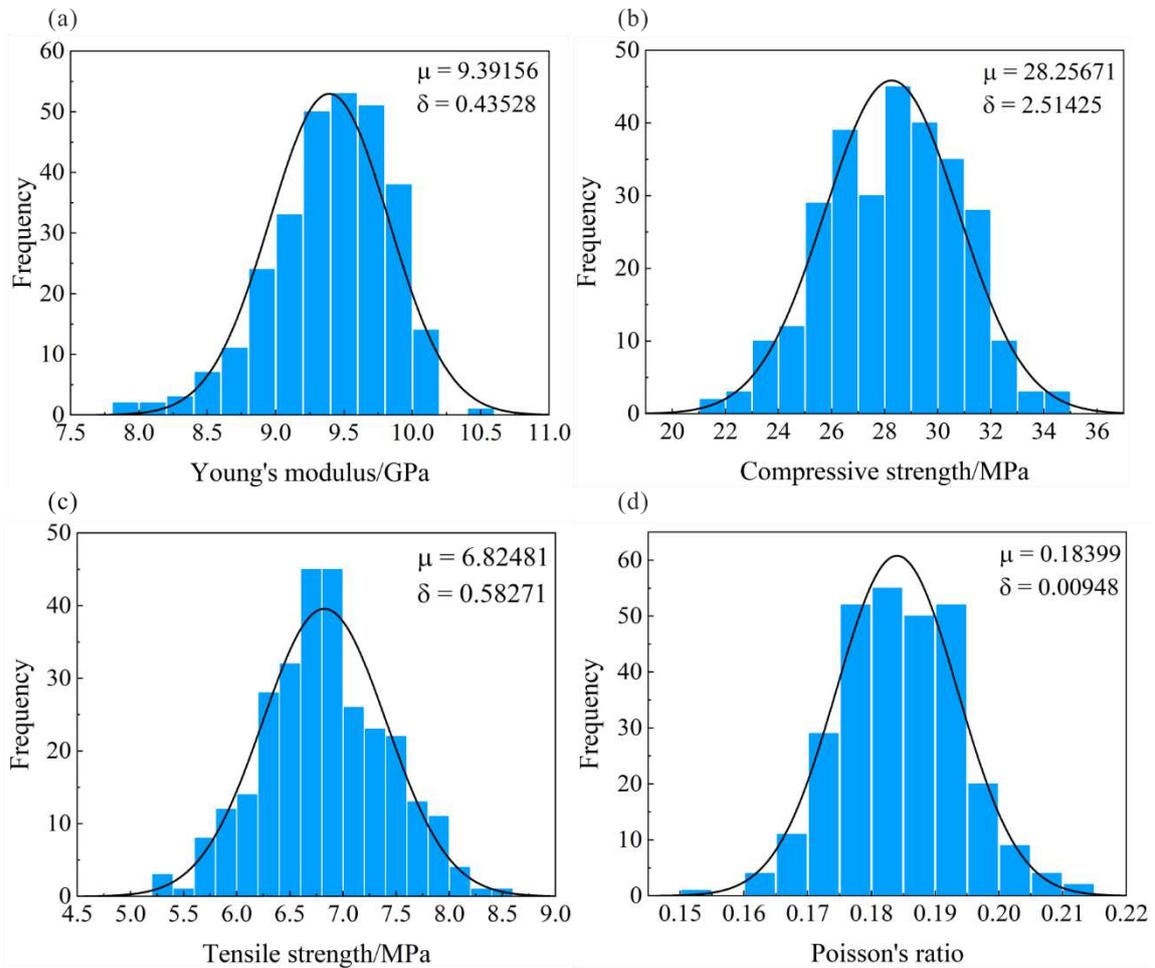
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Table 3 Normal test of stochastic simulation results of particle distribution

Items	Young's modulus	Compressive strength	Tensile strength	Poisson's ratio
Mean	9.39	28.26	6.82	0.184
Std. Deviation	0.435	2.51	0.583	0.009
Skewness, g_1	-0.636	-0.12	0.055	0.07
Skewness Std. Deviation, σ_{g1}	0.143	0.143	0.143	0.143
U test, u_1	-4.45	-0.84	0.38	0.49
Kurtosis, g_2	0.494	-0.42	-0.066	0.066

Kurtosis Std. Deviation, σ_{g2}	0.286	0.286	0.286	0.286
U test, u_2	1.73	-1.47	-0.23	0.23
LL (P)	0.015	0.2	0.063	0.2
S-W (P)	0	0.172	0.812	0.876
Normality	No	Yes	Yes	Yes

203



204

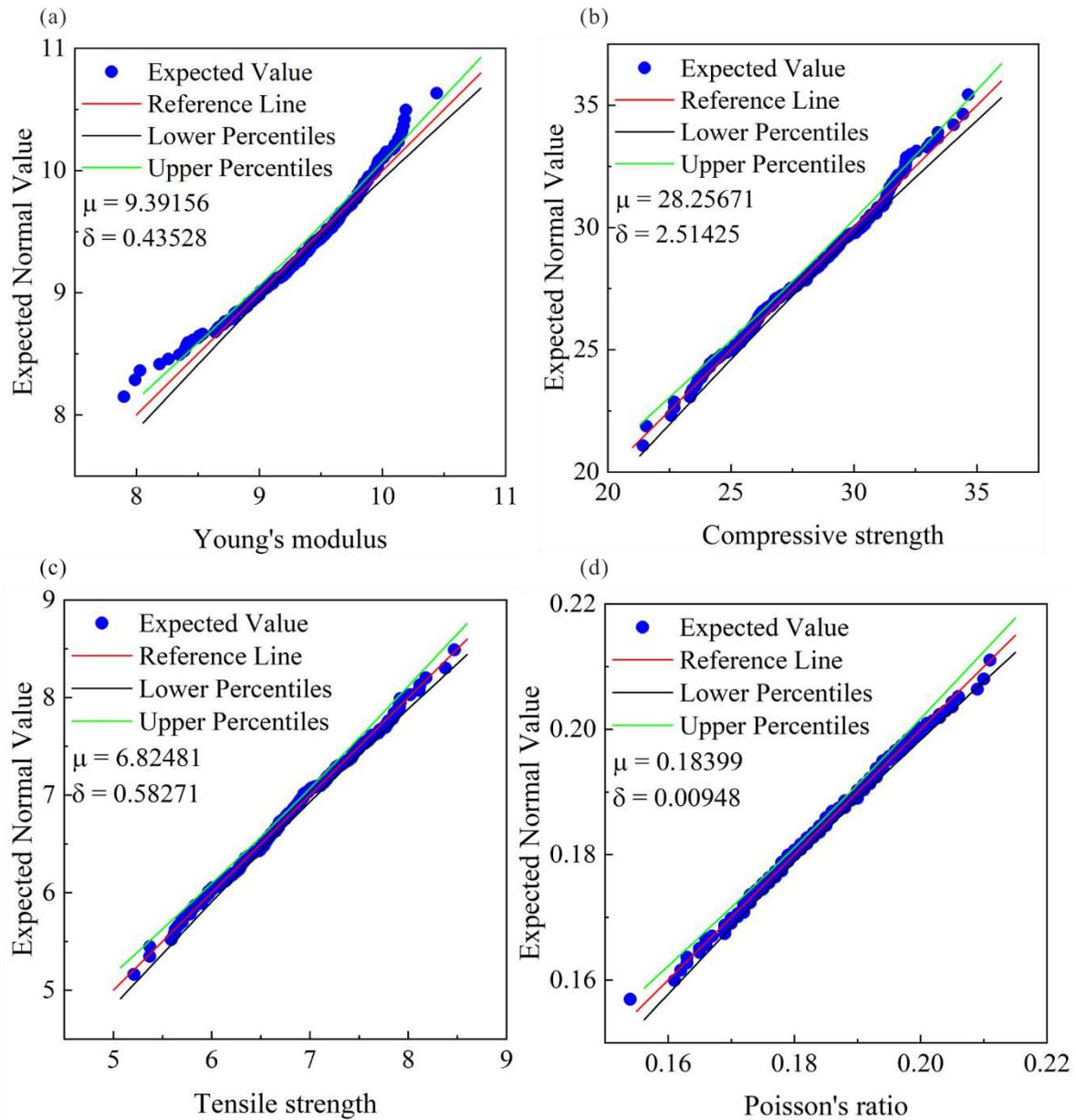
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Fig. 3 Histogram of the macroscopic property results with different particle distributions: (a) Young's

206

modulus; (b) compressive strength; (c) tensile strength; (d) Poisson's ratio.

207



208

209 Fig. 4 Q-Q diagram of the macroscopic property results with different particle distributions: (a) Young's

210 modulus; (b) Compressive strength; (c) Tensile strength; (d) Poisson's ratio

211

212 To determine the specific distributions for the results of Young's modulus, the raw data

213 that do not follow a standard normal distribution need to be converted. Commonly used

214 conversion methods are the logarithmic transformation, square root transformation and

215 reciprocal transformation (Nishida, 2010), as defined in the following:

216 $y = \ln(K - x)$

217 9.

218 $y = \sqrt{|(K - x)|}$

219 10.

220 $y = \frac{1}{K - x}$

221 11.

222

223 Where, K is a constant, x and y are the original and transformed data, respectively.

224

225 The coefficient K is obtained by letting the skewness of transformed data equal to zero.

226 After trial and error, the logarithmic transformation is used for the Young's modulus data. The

227 coefficient K for Young's modulus 11.384.

228

229 Normality tests are performed on the transformed data, and the results are shown in Table

230 4, Fig. 5 and Fig. 6. The U test values, the significance of LL test and S-W test of the Young's

231 modulus after the transformation meet the standard of normal distributions. Meanwhile, almost

232 all of the data points in the normal Q-Q diagram are within the range corresponding to the

233 confidence level. In summary, the transformed data of Young's modulus follow the normal

234 distribution, and the original data of Young's modulus follows negatively skewed distributions.

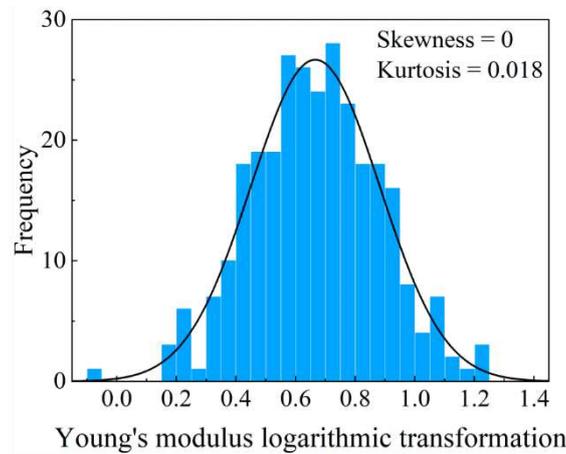
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Table 4 Results of normality test after data conversion

Items	Young's modulus
Conversion method	logarithmic

Skewness, g_1	0
Skewness Std. Deviation, σ_{g1}	0.143
U test, u_1	0
Kurtosis, g_2	0.018
Kurtosis Std. Deviation, σ_{g2}	0.286
U test, u_2	0.063
LL (P)	0.2
S-W (P)	0.969
Normality (after data conversion)	Yes

236

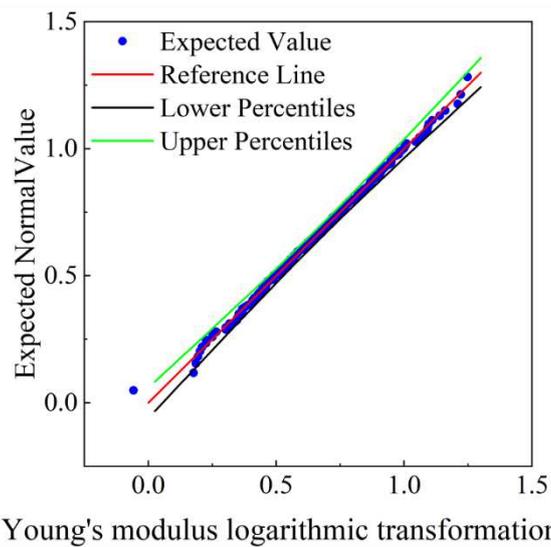


237

238

Fig. 5 Histogram of macroscopic property result after Young's modulus data conversion

239



240

241

Fig. 6 Q-Q graph of the macroscopic property result after Young's modulus data conversion

242

243 3.2 Determination of the minimum sample size for high-precision averages

244 It has been demonstrated that the randomness of particle distribution has a significant
245 effect on the results of macroscopic mechanical properties of the discrete element model. So in
246 model calibrations, the averages obtained from multiple calculations with different particle
247 distributions should be used, instead of the results from one calculation without considering
248 particle distributions. The approach to determine the number of computations (sample size) is
249 of significant. Apparently, the larger the sample size, the smaller the deviations of averages
250 (Naing, 2003); but in practice, due to the limitation of computing resource, it is impossible to
251 perform infinite calculations to obtain the true averages. Therefore, the correlation between the
252 sample size and the precision of the corresponding average values needs to be studied, then a
253 reasonable calculation number that balances the computing accuracy and efficiency can be
254 determine.

255

256 According to the fundamental theory of random sampling, the minimum sample size
257 required to obtain an average for a given precision can be determined according to the total
258 sample variance, allowable error (accuracy) and confidence (Naing, 2003):

259
$$n_{min} = \frac{Z^2 S^2}{\Delta_x^2}$$

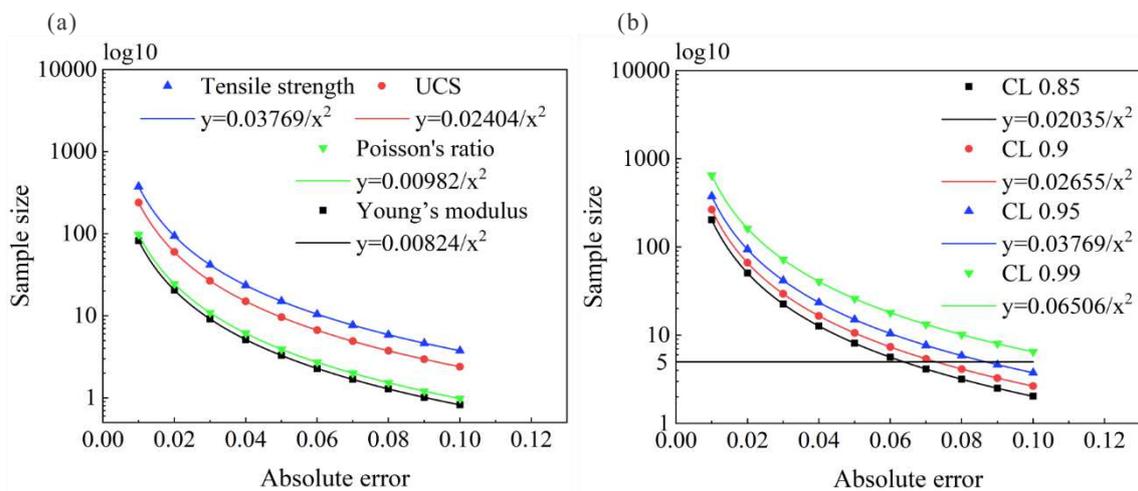
260 12.

261

262 The standard deviations of the population samples of each item can be found in Table 3.
263 The selection confidence is 95%. The minimum sample size of each macroscopic properties

264 under different accuracy are calculated According to Eq. 12, and the results are shown in Fig.
 265 7 (a). The results indicate that the minimum sample size becomes larger when the preset error
 266 decreases. The fitted curves are also shown in Fig. 7 (a); the minimum sample size for all
 267 macroscopic parameters are inversely proportional to the square of error. By comparing the
 268 minimum sample size of each item with the same precision, it can be found that the minimum
 269 sample size of tensile strength is always the largest. The confidence level also affects the
 270 minimum sample size. As Fig. 7(b) shows, at the same precision, the minimum sample size
 271 increases with the confidence level.

272



273

274 Fig. 7 Determination of the minimum sample size :(a) the minimum sample size of each item varies with
 275 the accuracy level when the confidence is 95%; (b) the minimum sample size of tensile strength with given
 276 accuracy level under different confidence levels

277

278 3.3 Verification of the "three in five tests for the mean" method

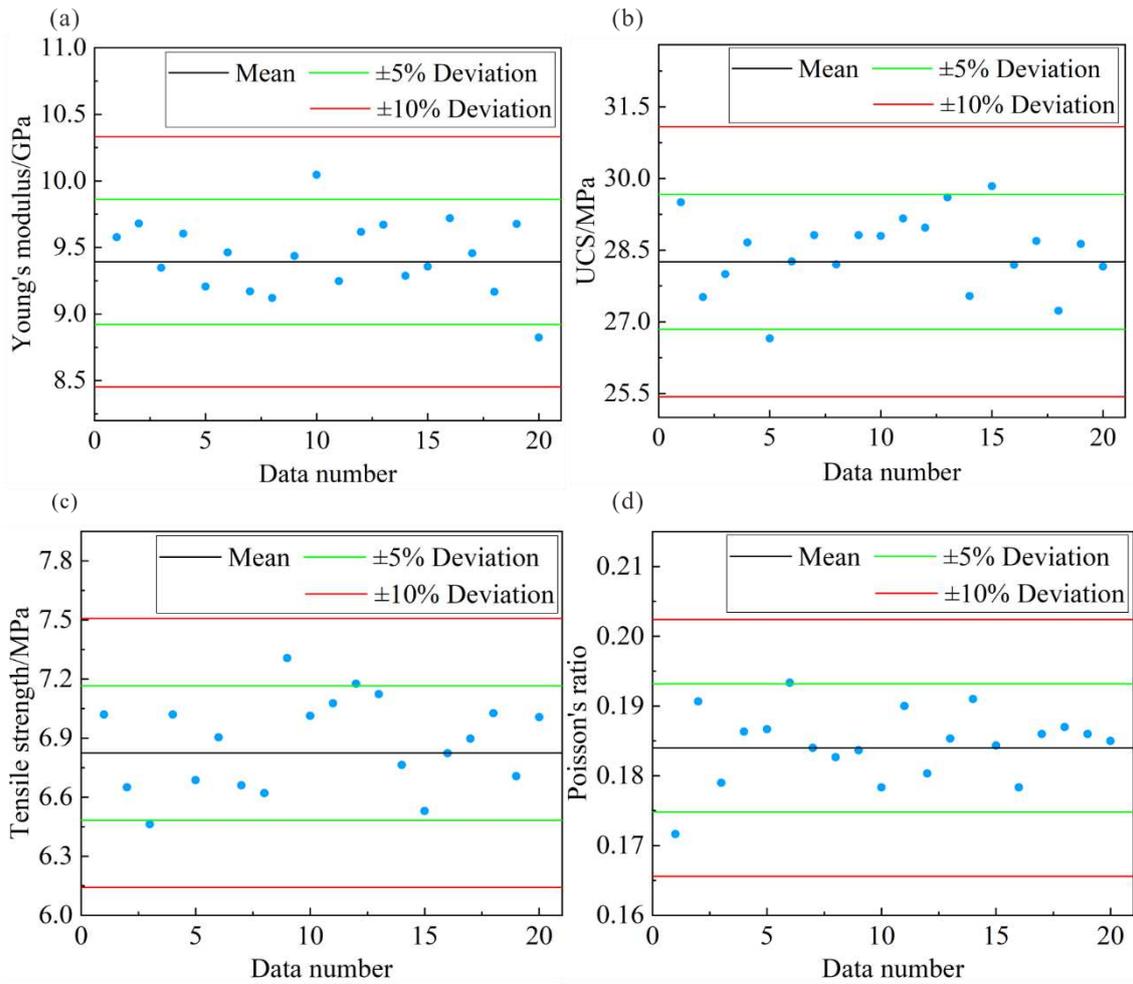
279 The "three in five tests for the mean" method (which is shortened as "three in five" method

280 in the following) is popular in the investigations involving stochastic problems. In this method,
281 each test will be repeated five times, and the middle three values are adopted to calculate the
282 average. To verify the applicability of the “three in five” method in calculating the averages
283 that used for calibrations, five data points of macroscopic properties are randomly selected
284 from the sample, then the maximum and minimum values are removed and the average are
285 calculated according to the remaining three values. The sampling process is repeated for 20
286 times, and the corresponding averages are shown in Fig. 8.

287

288 All the results (Fig. 8) of Young's modulus, compressive strength, tensile strength and
289 Poisson's ratio show a certain degree of dispersion, but the relative errors of the averages
290 obtained by the “three in five” method are largely smaller $\pm 5\%$. The maximum error in Fig. 8
291 is about 7.5%. As shown by Fig. 7 (b), when sample size is five, the relative error of the average
292 is about 8.7% which is larger than that of the average obtained by the “three in five” method
293 where the effects of maximum and minimum are eliminated. In summary, the "three in five"
294 method works well for the problem of calculating the averages that used for calibrations.

295



296

297 Fig. 8 Error analysis of the averages obtained by the "five choose three" method : (a) Young's modulus; (b)

298

compressive strength; (c) tensile strength; (d) Poisson's ratio.

299

300 4 Conclusion

301

In this paper, the statistical rule of the influence of particle distributions on the

302

macroscopic mechanical property discreteness of the particle flow model is studied. The major

303

conclusions are as follows:

304

305

a. The particle distributions have a significant effect on the macroscopic mechanical

306

properties of particle flow model, and the simulation results of compressive strength, tensile

307 strength and Poisson's ratio with different particle distributions follows normal distributions,
308 while that of Young's modulus follow negative skewness distributions. Therefore, the averages
309 obtained from multiple calculations with different particle distributions should be used for
310 model calibrations, instead of the results from one calculation without considering particle
311 distributions.

312

313 b. The minimum sample size required to obtain averages of macroscopic mechanical
314 properties with a given precision level is inversely proportional to the square of precision.

315

316

317 c. The "three in five" method (calculating five times with different particle distributions
318 and calculate the average value after removing the maximum and minimum) is adopted to
319 obtain the averages of macroscopic mechanical properties that used for model calibrations. The
320 deviations of the averages provided by this method is largely within the range of $\pm 5\%$ while
321 the maximum of deviations is not over $\pm 10\%$, suggesting that the "three in five" method is
322 effective.

323

324 **Acknowledgement**

325 The authors would like to thank the support from National Natural Science Foundation of
326 China (Grant No.52005419), Key research and development project of Sichuan
327 Province(21ZDYF3658),Major Scientific and Technological Innovation Projects in Chengdu

328 (2019-YF08-00100-GX)and China postdoctoral science foundation (Grant Number
329 2019M663898XB). China railway engineering services co. LTD is also acknowledged.

330

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452

453 **Figure captions**

454 Fig. 1 Particle flow models for simulating uniaxial tests and typical results: (a) model for
455 uniaxial compression tests; (b) crack distribution after uniaxial compression tests; (c) model
456 for uniaxial tensile tests; (d) crack distribution after uniaxial tensile tests

457 Fig. 2 Stress-strain response: (a) uniaxial compression tests; (b) uniaxial tensile tests

458 Fig. 3 Histogram of the macroscopic property results with different particle distributions: (a)
459 Young's modulus; (b) compressive strength; (c) tensile strength; (d) Poisson's ratio.

460 Fig. 4 Q-Q diagram of the macroscopic property results with different particle distributions: (a)
461 Young's modulus; (b) Compressive strength; (c) Tensile strength; (d) Poisson's ratio

462 Fig. 5 Histogram of macroscopic property result after Young's modulus data conversion

463 Fig. 6 Q-Q graph of the macroscopic property result after Young's modulus data conversion

464 Fig. 7 Determination of the minimum sample size :(a) the minimum sample size of each item
465 varies with the accuracy level when the confidence is 95%; (b) the minimum sample size of
466 tensile strength with given accuracy level under different confidence levels

467 Fig. 8 Error analysis of the averages obtained by the "five choose three" method : (a) Young's
468 modulus; (b) compressive strength; (c) tensile strength; (d) Poisson's ratio.

Figures

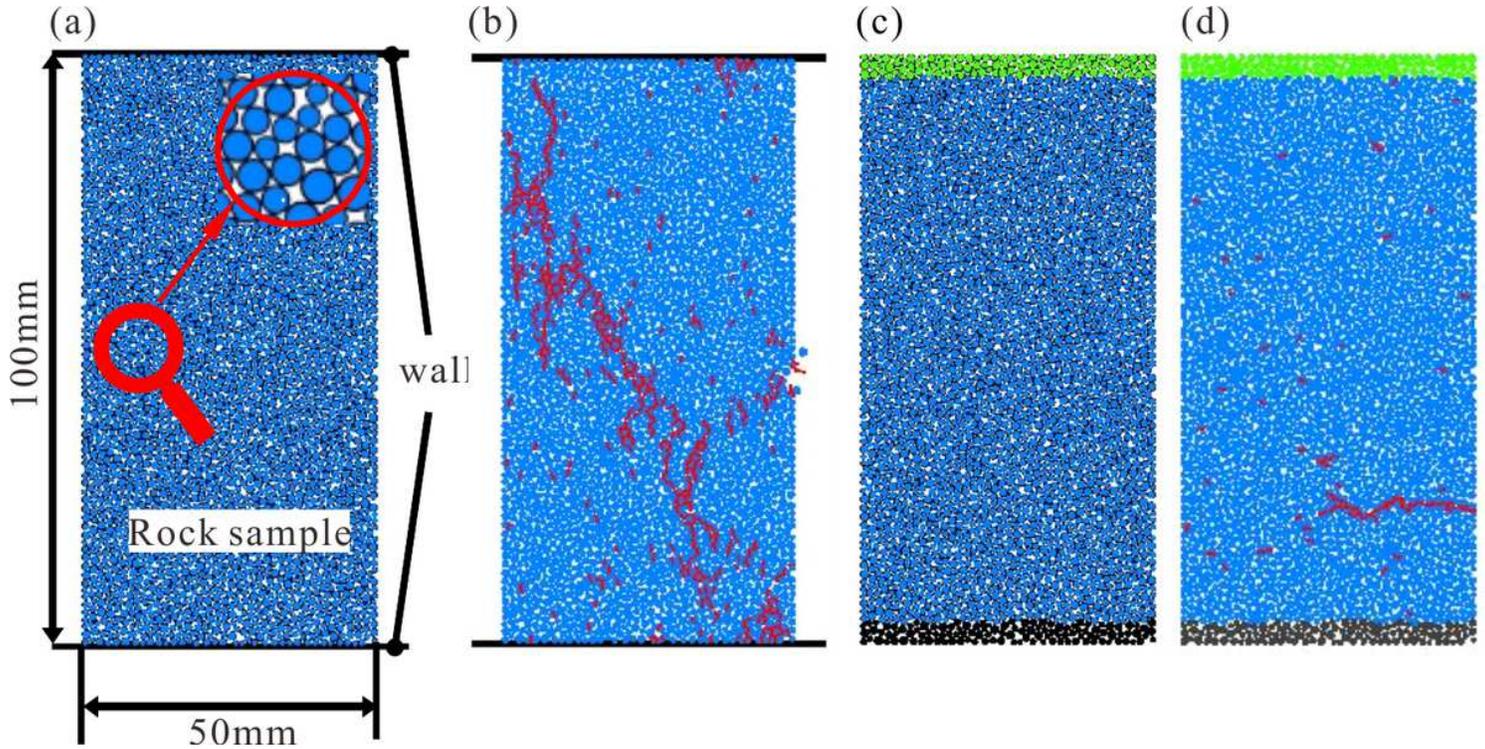


Figure 1

Particle flow models for simulating uniaxial tests and typical results: (a) model for uniaxial compression tests; (b) crack distribution after uniaxial compression tests; (c) model for uniaxial tensile tests; (d) crack distribution after uniaxial tensile tests

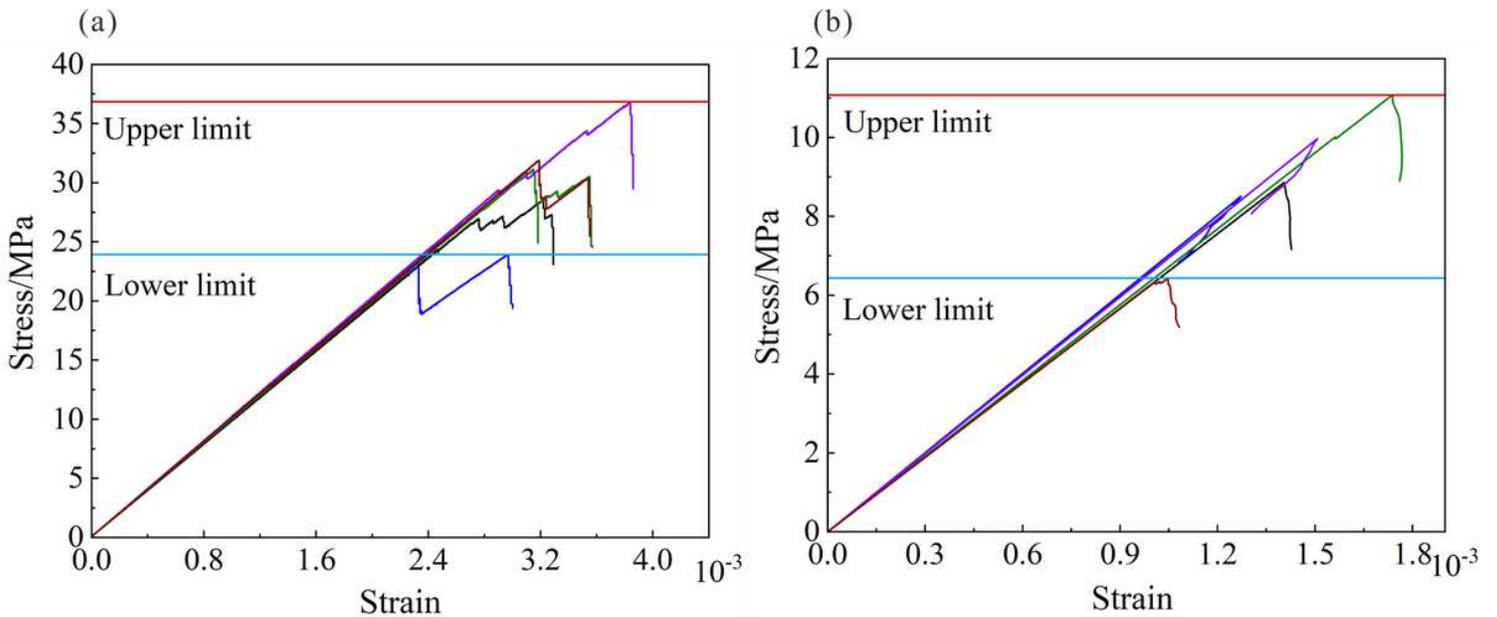


Figure 2

Stress-strain response: (a) uniaxial compression tests; (b) uniaxial tensile tests

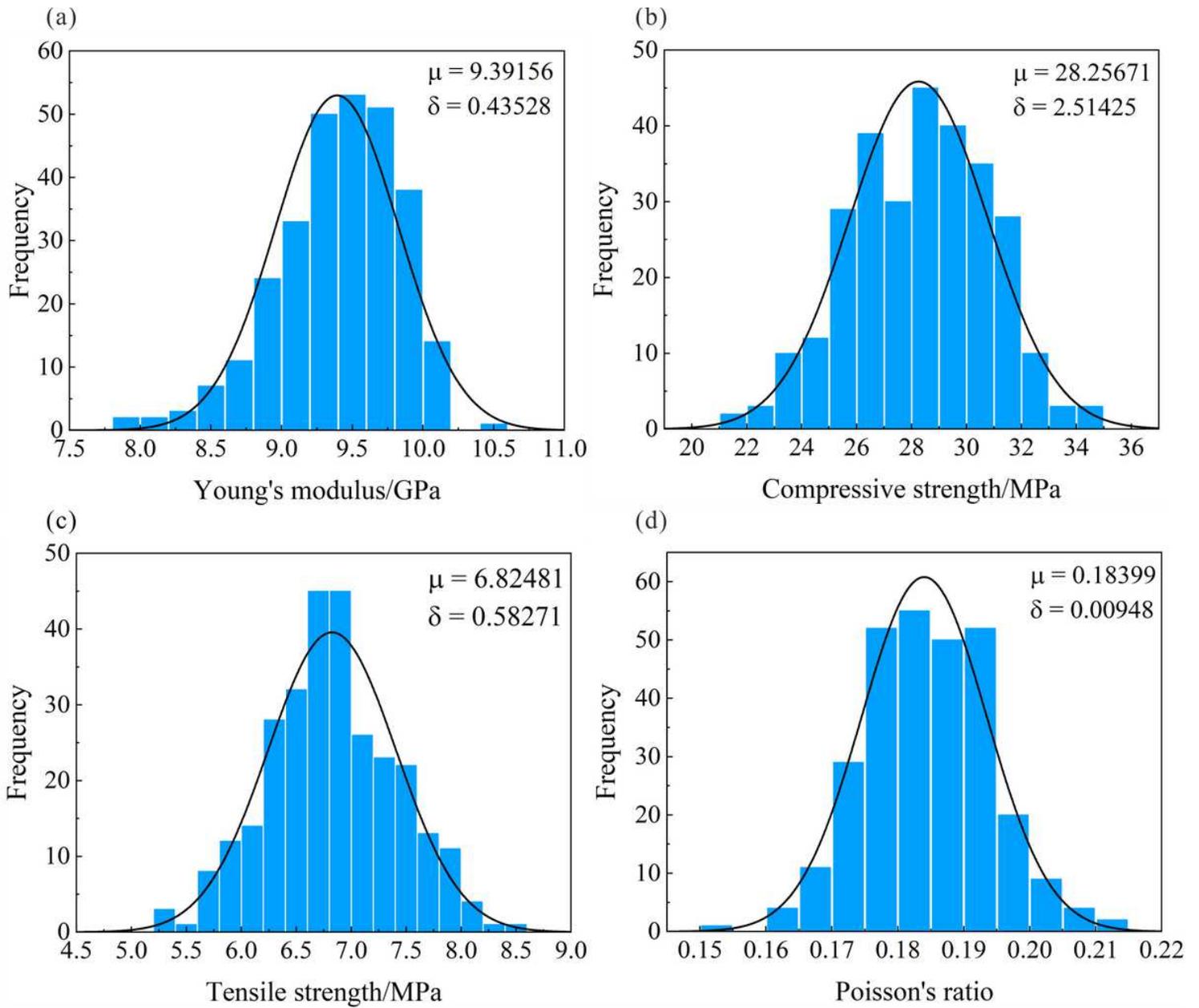


Figure 3

Histogram of the macroscopic property results with different particle distributions: (a) Young's modulus; (b) compressive strength; (c) tensile strength; (d) Poisson's ratio.

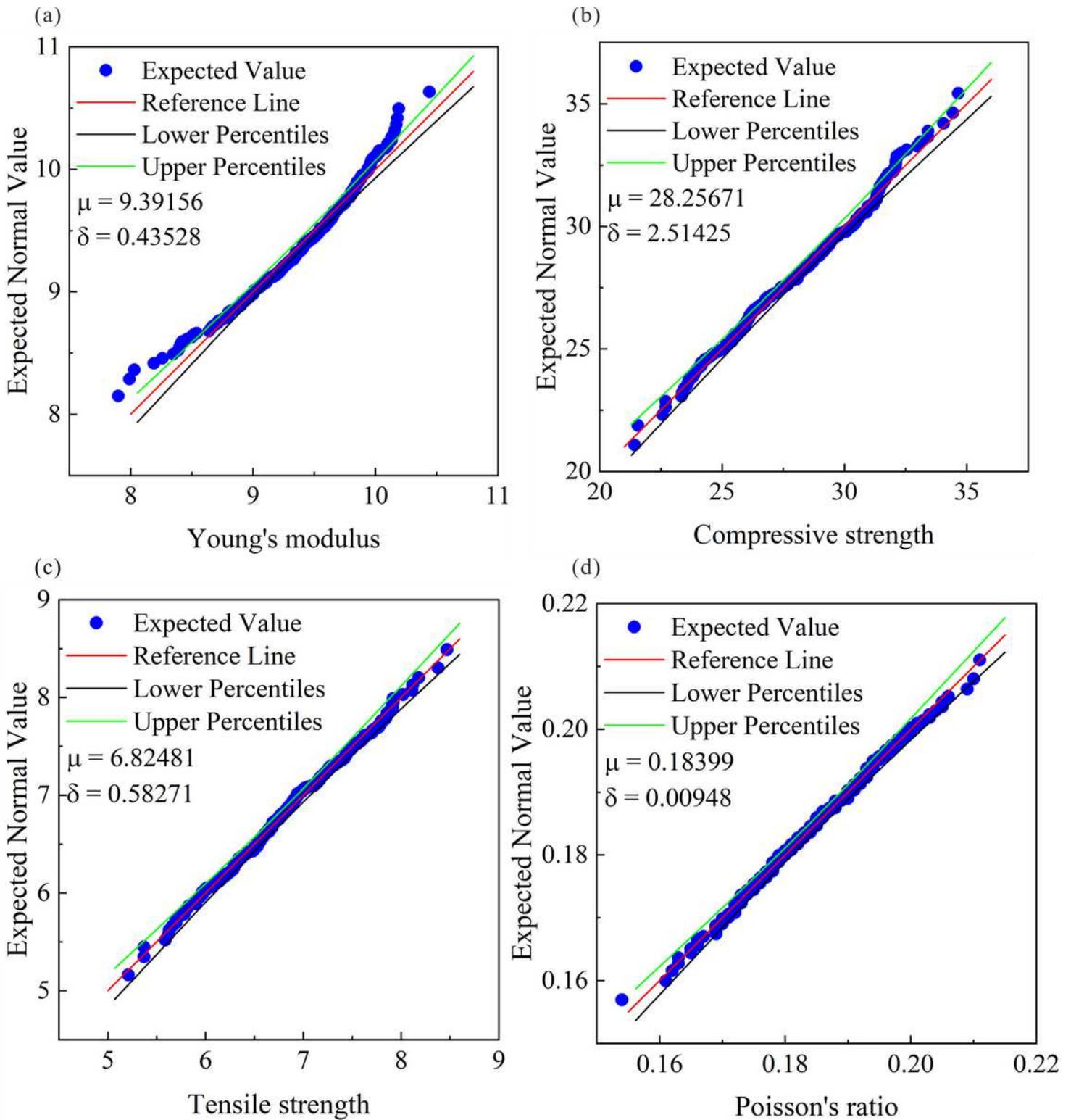


Figure 4

Q-Q diagram of the macroscopic property results with different particle distributions: (a) Young's modulus; (b) Compressive strength; (c) Tensile strength; (d) Poisson's ratio

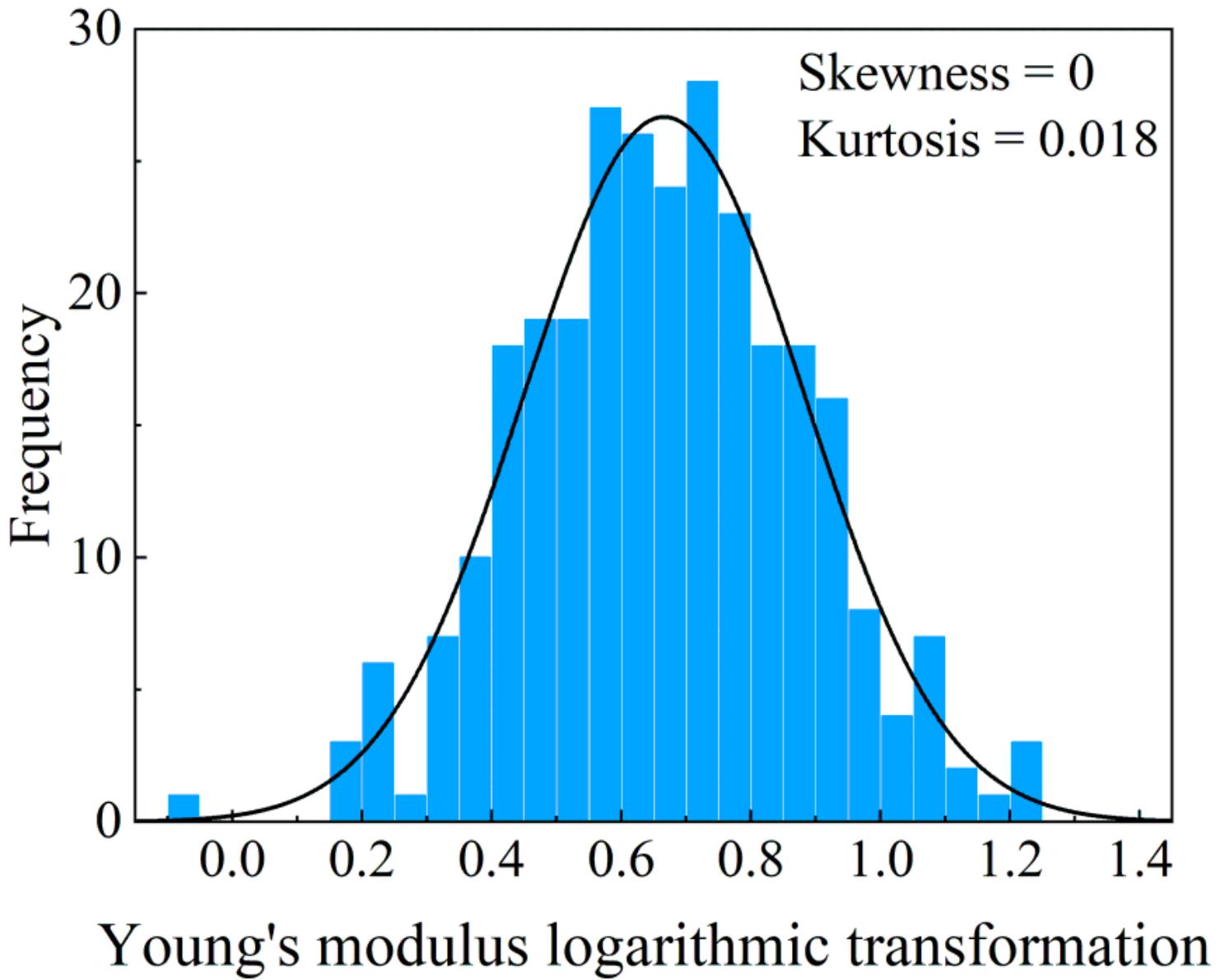
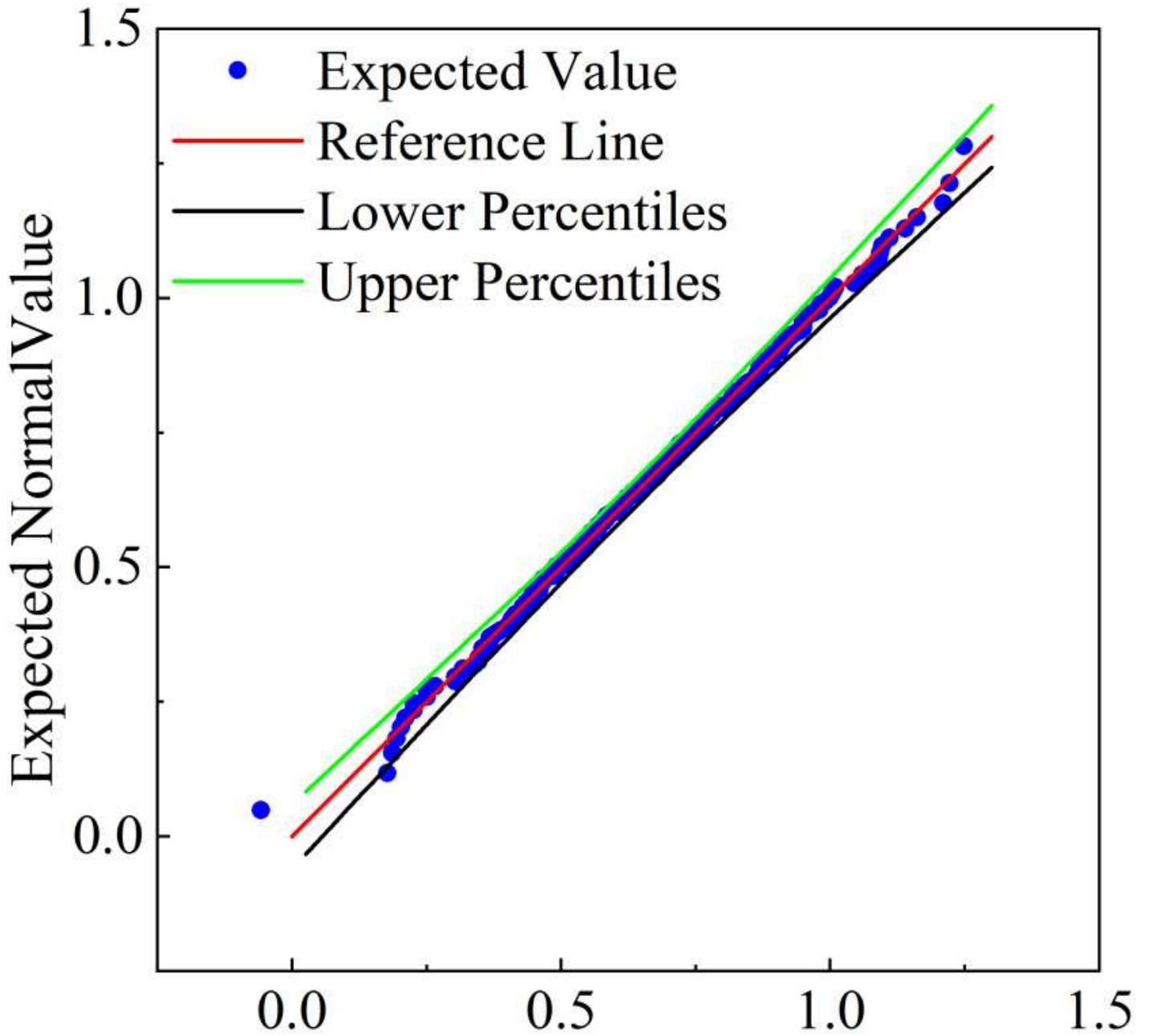


Figure 5

Histogram of macroscopic property result after Young's modulus data conversion



Young's modulus logarithmic transformation

Figure 6

Q-Q graph of the macroscopic property result after Young's modulus data conversion

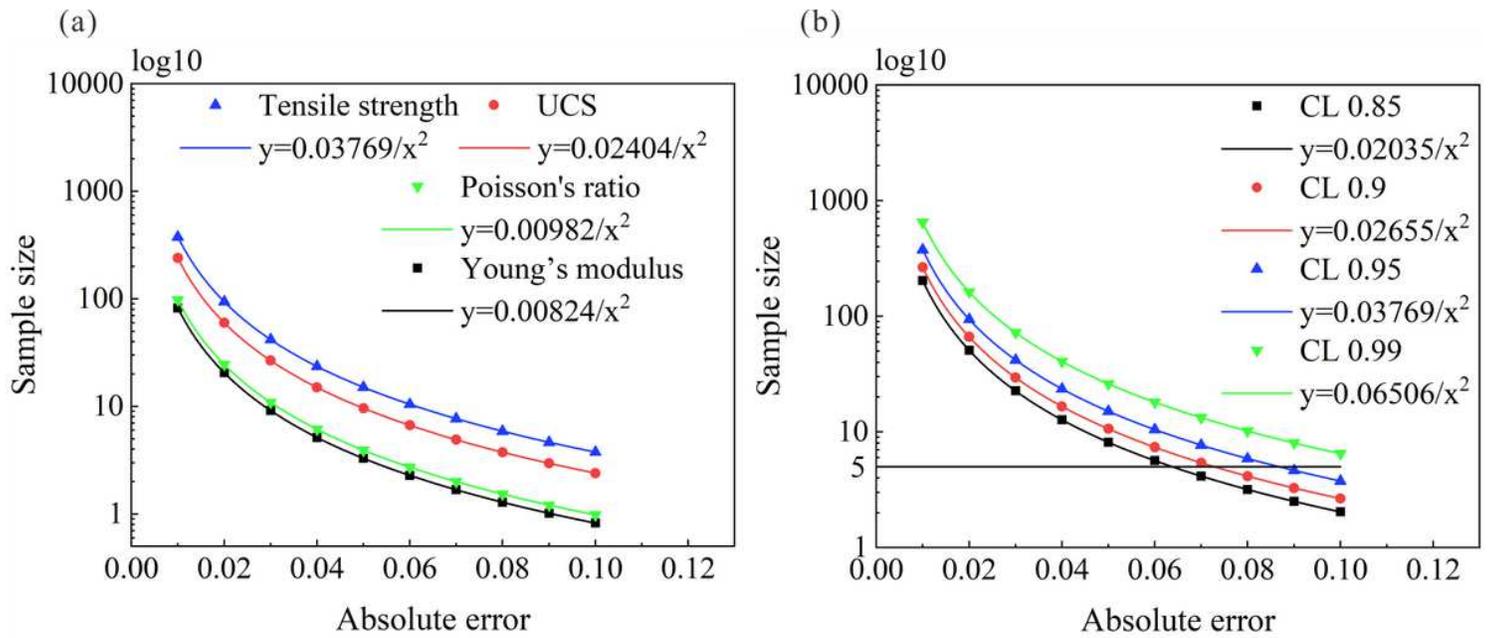


Figure 7

Determination of the minimum sample size :(a) the minimum sample size of each item varies with the accuracy level when the confidence is 95%; (b) the minimum sample size of tensile strength with given accuracy level under different confidence levels

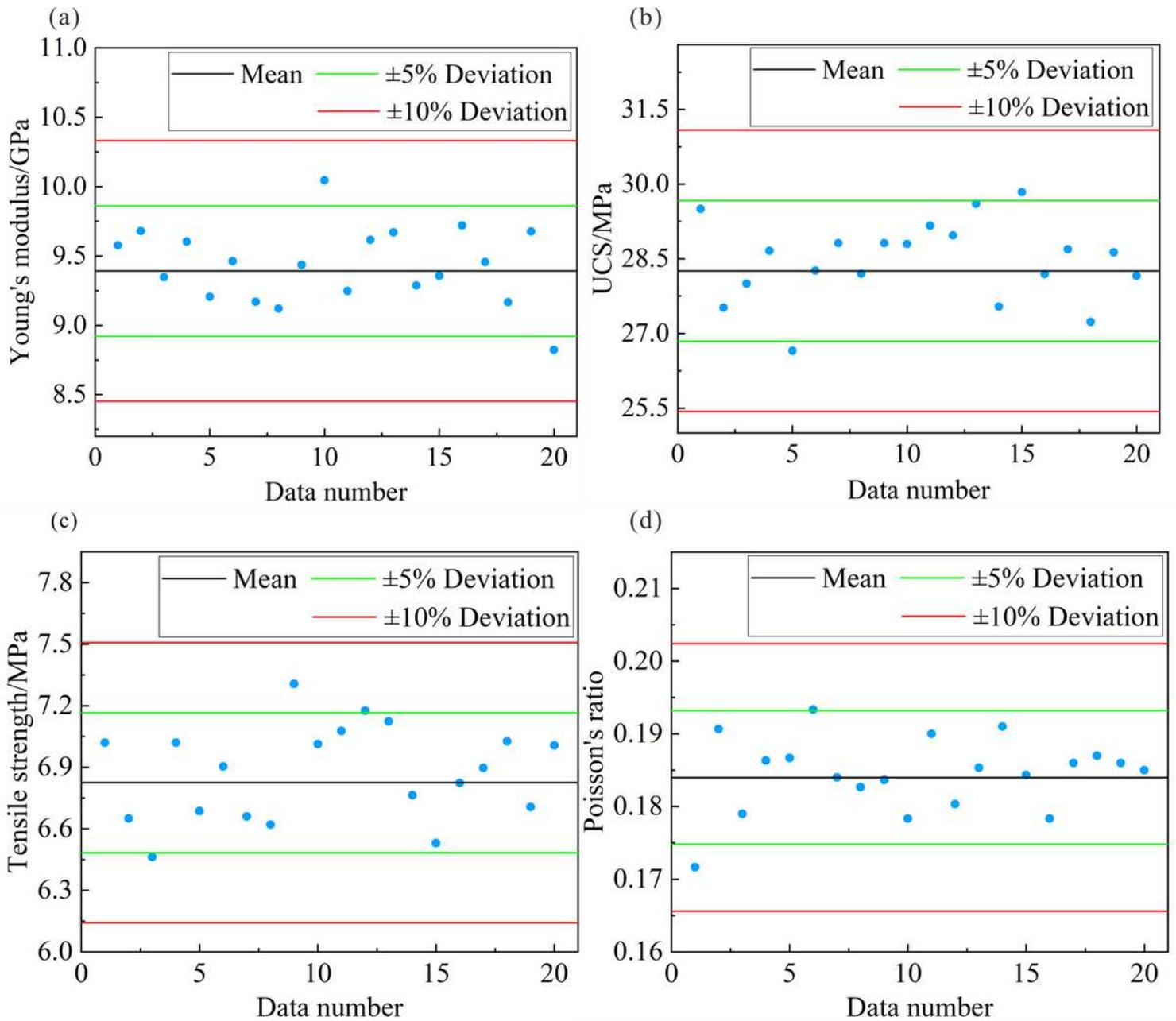


Figure 8

Error analysis of the averages obtained by the "five choose three" method : (a) Young's modulus; (b) compressive strength; (c) tensile strength; (d) Poisson's ratio.