Parameter estimation approach for particle flow model of rockfill materials using response surface method

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Abstract

Particle flow code (PFC) is widely used to model deformation and stress states of rockfill materials. The accuracy of numerical modelling with PFC is dependent upon the model parameter values. How to accurately determine model parameters remains one of the main challenges. In order to determine model parameters of particle flow model of rockfill materials, some triaxial compression experiments are performed, and the inversion procedure of model parameters based on response surface method is proposed. Parameters of particle flow model of rockfill materials are determined according to observed data in triaxial compression tests for rockfill materials. The investigation shows that the normal stiffness, tangent stiffness and friction coefficient of rockfill materials will slightly increase with increase of confining pressure in triaxial compression tests. The experiments in laboratory show that the proposed inversion procedure behaves higher computing efficiency and the forecasted stress-strain relations agree well with observed values.

Keywords: micromechanical model, rockfill materials, parameter inversion, triaxial compression tests, response surface method

1. Introduction

Rockfill materials are widely used to construct dams. The deformation characteristics of rockfill materials commonly are numerically simulated by distinct element method and PFC software. The accuracy of numerical modelling with PFC is dependent upon the model parameter values. How to accurately determine model parameters remains one of the main challenges. Some researchers have tried to determine the micromechanical model parameters of granular materials experimentally. Masson performed a set of distinct element simulations of the filling and the discharge of a plane rectangular silo with variable values of particle mechanical parameters. The analysis of the influence of friction and stiffness of contacts showed that these parameters played a major role in the flow kinematics and in the stress field during filling and discharge processes [Masson and Martinez (2000)]. Bagherzadeh developed a novel approach for the two-dimensional numerical simulation of the phenomenon in rockfill using combined DEM and FEM. All particles were simulated by the discrete element method as an assembly and after each step of DEM analysis, each particle was separately modeled by FEM to determine its possible breakage [Bagherzadeh et al. (2011)]. Hosseininia presented a model to simulate the breakage of two-dimensional polygon-shaped particles. In the model, each uniform (uncracked) particle was replaced with smaller inter-connected sub-particles which are bonded with each other [Hosseininia and Mirghasemi (2006)].

Renzo performed a mathematical modification of Mindlin's tangential solution and demonstrated formally its advantages with respect to the commonly used model [Renzo and Maio (2005)]. Coetzee presented a method for determining the parameters of cohesionless granular material. The particle size and density were directly measured and modeled. The particle shapes were modeled using two to four spheres clumped together. The remaining unknown parameter values were determined using confined compression tests and angle of repose tests [Coetzee et al. (2010)]. Koyama proposed a numerical procedure to determine the equivalent micro-mechanical properties of intact rocks using a stochastic representative elementary volume (REV) concept and a particle mechanics approach. More than 200 models were generated in square regions with side lengths varying from 1 to 10 cm, using the Monte Carlo simulation technique [Koyama and Jing (2007)]. Kulatilake performed laboratory experiments and numerical simulations to study the behavior of jointed blocks of model material under uniaxial loading. The effect of joint geometry parameters on the uniaxial compressive strength of jointed blocks was investigated [Kulatilake et al. (2001)]. Each particle has material parameters (micro-parameters) that influence the particle macro-behaviors. The accuracy of PFC model depends on the micro-parameters of model. How to accurately determine PFC model parameters remains one of the main challenges.

PFC^{2D} models the movement and interaction of circular particles by the distinct element method (DEM), as described by Cundall and Strack (1979). The overall constitutive behavior of a material is simulated in PFC^{2D} by associating a simple constitutive model with each contact. The constitutive model acting at a particular contact consists of three parts: a stiffness model, a slip model, and a bonding model. The stiffness model provides an elastic relation between the contact force and relative displacement. The slip model enforces a relation between shear and normal contact forces such that the two contacting balls may slip relative to one another. The bonding model serves to limit the total normal and shear forces that the contact can carry by enforcing bond-strength limits. González-Montellano performed the experimental to determine values for several of the microscopic properties-the particle density, modulus of elasticity, particle-wall coefficient of restitution, particle-particle coefficient of restitution, and the particle-wall coefficient of friction-of maize grains and olives, required for use in DEM simulations [González-Montellano et al. (2012)]. Yoon developed a new approach for calibrating contact-bonded particle models using 'experimental design' and 'optimization' in uniaxial compression simulation. These were applied to calculate an optimum set of microparameters used in generation of models to be tested in uniaxial compression simulations [Yoon (2007)]. Belheine calibrated the micro-mechanical properties of the numerical material using numerical triaxial tests in order to match the macroscopic response of the real material. Numerical simulations were carried out under the same conditions as the physical experiments. The pre-peak, peak and post-peak behaviors of the numerical material were studied [Belheine et al. (2009)]. Chen investigated the failure mechanism and the limit support pressure of a tunnel face in dry sandy ground by using discrete element method. The contact parameters of the dry sand particles were obtained by calibrating the results of laboratory direct shear tests. A series of three-dimensional DEM models for different ratios of the cover depth to the diameter of the tunnel were then built to simulate the process of tunnel face failure [Chen et al. (2011)]. Deluzarche proposed a methodology to define the resistance of the 2D particles so that the same probability of breaking blocks may be reproduced as in a 3D material. The model used the discrete element code PFC^{2D} and considered breakable clusters of 2D balls. The different parameters were determined from experimental data obtained from laboratory tests performed on rock blocks [Deluzarche and Cambou (2006)]. Alaei simulated single crushing tests and triaxial tests on the Purulia dam's material to validate the presented model for rockfill material. The obtained results demonstrated the accuracy of the adopted model and the model's capability for considering a rockfill material's strength, deformation and crushing behaviour [Alaei and Mahboubi (2012)]. Even if some procedures has been proposed to determine micromechanical parameters of rockfill materials, the common drawback of these estimating procedures lies in lower fitting and predicting precision. Response surface methodology is a collection of statistical and mathematical techniques useful for developing, improving, and optimizing processes in which a response of interest is influenced by several variables and the objective is to optimize this response. Response surface methodology has been widely applied in inverse solution of soil-water transport model parameters [Saha et al. (2010)], parameter optimization [Muthuvelayudham and Viruthagiri (2010)], nutritional parameter optimization [Kunamneni et al. (2005)]. The aim of the paper is to propose a new procedure for determining PFC model parameters of rockfill materials from triaxial compression tests and to validate effectiveness of proposed inversion approach through experiments in laboratory.

2. Numerical simulations for triaxial compression tests using PFC software

PFC model is based on the simulations of the motion of granular material as separate particles. Using the soft particle approach, each particle contact is modeled with a linear spring both in the contact normal direction and contact tangential direction, as shown in Figure 1. The particles are allowed to overlap and the amount of overlap is used in combination with the spring stiffness to compute the contact force components.

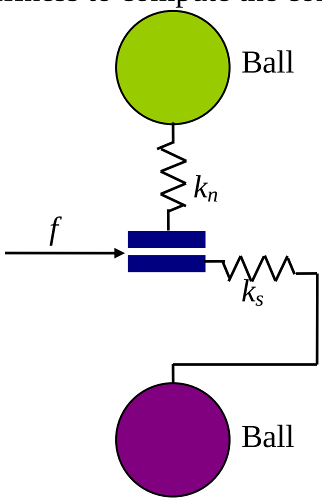

Figure 1. DEM contact model

The normal stiffness of a particle is secant stiffness. The relation between normal force and normal displacement is expressed as follows

$$F_n = k_n U_n \quad (1)$$

Where F_n denotes total normal force, k_n denotes normal stiffness, U_n denotes total normal displacement. The shear stiffness of a particle is a tangent stiffness. The relation between increment of tangent force and increment of tangent displacement is expressed as follows

$$\Delta F_s = -k_s \Delta U_s \quad (2)$$

Where ΔF_s denotes the increment of shear force, k_s denotes tangent stiffness, ΔU_s denotes the increment of shear displacement.The slip model is defined by the friction coefficient at the contact f [dimensionless], where f is taken to be the minimum friction coefficient of the two contacting entities.

In order to determine the model parameters of rockfill materials, some triaxial compression tests of rockfill materials are performed in laboratory. The largest size of rockfill particles is 100mm, as shown in Figure 2. The smallest size is 0.1mm. The diameter of test model is 300mm. The height is 700mm, as shown in Figure 3. Variation of deviatoric stress (principal stress difference: σ_1-σ_3) versus axial strain in triaxial compression test of rockfill materials is depicted in Figure 4. σ_1 is major stress (axial stress), and σ_3 is minor stress (confining pressure). These test data are available for parameter estimation of PFC model of rockfill materials.

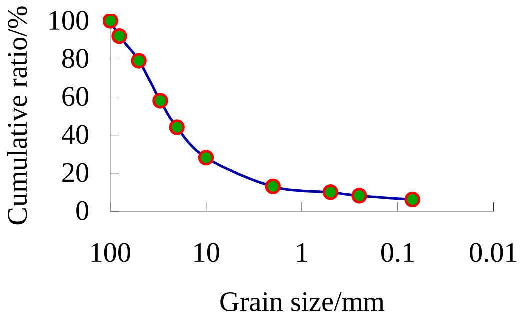

Figure 2. Particle size distribution for rockfill materials

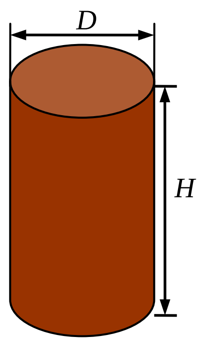

Figure 3. Triaxial compression test of rockfill materials

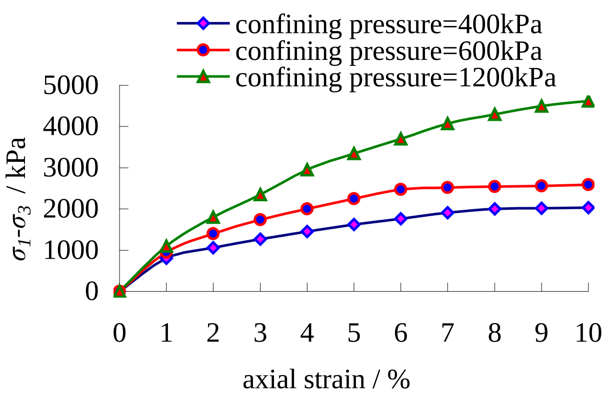

Figure 4. Variation of deviatoric stress versus axial strain in triaxial compression test of rockfill materials

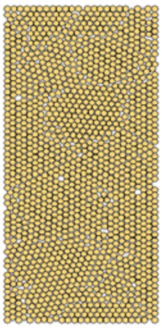

Figure 5. Simplified PFC^{2D} model of triaxial compression test of rockfill materials

After taking into account of symmetrical characteristic of triaxial compression test model, PFC model is simplified into two dimensions for simulating triaxial compression test of rockfill materials, as shown in Figure 5. The radius of rockfill particle in PFC^{2D} model is approached as 20mm according to the average radius of rockfill particle. Influences of normal stiffness, tangent stiffness and friction coefficient of rockfill materials on stress-strain relation are simulated with PFC model, as shown in Figure 6, 7 and 8.

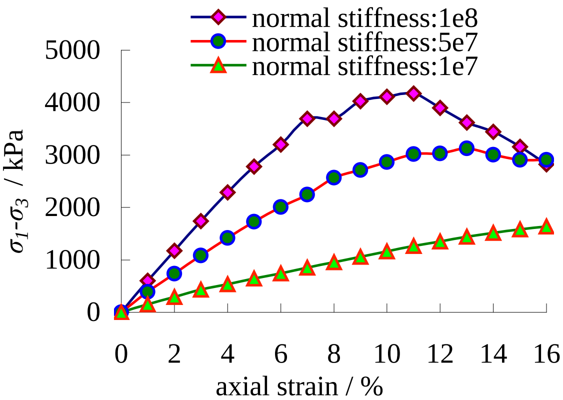

Figure 6. Influence of normal stiffness of rockfill materials on stress-strain relations (Confining pressure 1200kPa)

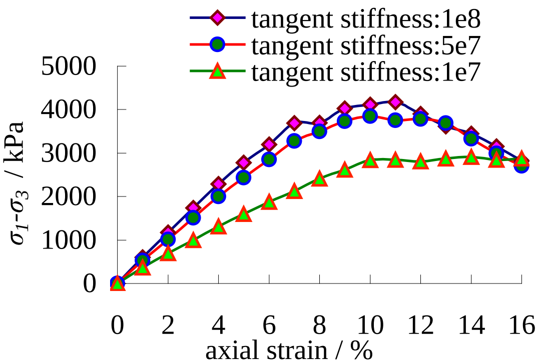

Figure 7. Influence of tangent stiffness of rockfill materials on stress-strain relations (Confining pressure 1200kPa)

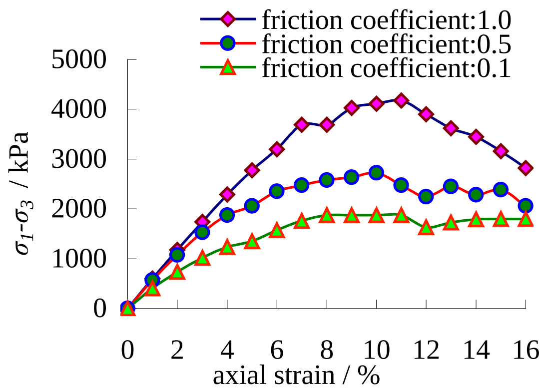

Figure 8. Influence of friction coefficient of rockfill materials on stress-strain relations (Confining pressure 1200kPa)

3. Parameter inversion procedures for PFC model using response surface method

Based on the response surface method, the relation between unknown PFC model parameters of rockfill materials and deviatoric stress in triaxial compression test is approached as [Rosa et al. (2009); Bas and Boyaci (2007)].

$$s_k(\bar{\mathbf{x}}) = a + \sum_{i=1}^{3} b_i \bar{x}_i + \sum_{i=1}^{3} c_i \bar{x}_i^2 \tag{3}$$

Where $s_k(\bar{\mathbf{x}})$ is principal stress difference (σ_1-σ_3) at loading step k, a, b_i and c_i are unknown coefficients, $\bar{\mathbf{x}}$ is unknown model parameter vector after dimensionless procedure.

$$\bar{\mathbf{x}} = \{\bar{x}_1, \bar{x}_2, \bar{x}_3\}^T = \{\bar{k}_n, \bar{k}_s, \bar{f}\}^T \tag{4}$$

$$\bar{k}_n = \frac{k_n}{\tilde{k}_n}, \bar{k}_s = \frac{k_s}{\tilde{k}_s}, \bar{f} = \frac{f}{\tilde{f}} \tag{5}$$

Where $\tilde{k}_n$, $\tilde{k}_s$ and $\tilde{f}$ denote initial evaluating values of model parameters according to prior to information.

Taking the first loading step as an example, the left items of following equations can be calculated by simulations using PFC^{2D} software under the given model parameter combinations

$$s_1^1(\bar{\mathbf{x}}) = s(\bar{k}_n, \bar{k}_s, \bar{f}) \tag{6}$$

$$s_1^2(\bar{\mathbf{x}}) = s(\bar{k}_n + \Delta\bar{k}_n, \bar{k}_s, \bar{f}) \tag{7}$$

$$s_1^3(\bar{\mathbf{x}}) = s(\bar{k}_n - \Delta\bar{k}_n, \bar{k}_s, \bar{f}) \tag{8}$$

$$s_1^4(\bar{\mathbf{x}}) = s(\bar{k}_n, \bar{k}_s + \Delta\bar{k}_s, \bar{f}) \tag{9}$$

$$s_1^5(\bar{\mathbf{x}}) = s(\bar{k}_n, \bar{k}_s - \Delta\bar{k}_s, \bar{f}) \tag{10}$$

$$s_1^6(\bar{\mathbf{x}}) = s(\bar{k}_n, \bar{k}_s, \bar{f} + \Delta\bar{f}) \tag{11}$$

$$s_1^7(\bar{\mathbf{x}}) = s(\bar{k}_n, \bar{k}_s, \bar{f} - \Delta\bar{f}) \tag{12}$$

Where $\Delta\bar{k}_n = 0.1$, $\Delta\bar{k}_s = 0.1$, $\Delta\bar{f} = 0.1$, s_1^i denotes principal stress difference computed in the first loading case under *i*-th parameter combination, which is computed by using PFC^{2D} software. There exist 7 unknown coefficients and 7 equations. So, the 7 unknown coefficients in response surface functions in the first loading case can be determined by solving linear equation set with MATLAB software. The unknown coefficients in response surface functions for other loading steps may be deduced by analogy.

Initial evaluating parameter values of PFC model of rockfill materials are listed in Table 1, where ρ denotes particle density, which is a known constant, σ_c denotes confining pressure in triaxial compression test.

Table 1. Initial evaluating parameter values of PFC model of rockfill materials

$\tilde{k}_n$ / N/m	$\tilde{k}_s$ / N/m	$\tilde{f}$	ρ / kg/m^3	σ_c / kPa
8.0e7	8.0e7	0.9	2800	400
1.2e8	1.2e8	0.9	2800	600
1.4e8	1.4e8	1.0	2800	1200

After performing a lot of numerical simulations for triaxial compression test with PFC software, the coefficients of response surface functions for every load step under different confining pressure are computed and listed in Table 2, 3 and 4.

Table 2. Coefficients of response surface functions for every load step (Confining pressure 400kPa)

Load step	a	b_1	b_2	b_3	c_1	c_2	c_3
1	-26.0	-1505.0	870.0	1230.0	850.0	-400.0	-600.0
2	-1255.0	-2800.0	2625.0	3515.0	1600.0	-1250.0	-1650.0
3	-120.0	-3325.0	685.0	4040.0	1850.0	-250.0	-1800.0
4	1793.0	2870.0	-5005.0	-1260.0	-600.0	2550.0	900.0
5	6447.0	-12430.0	1370.0	-155.0	6500.0	-700.0	450.0
6	9443.0	-12030.0	-4455.0	-720.0	6400.0	2250.0	800.0
7	-4291.0	3205.0	5305.0	1240.0	-950.0	-2750.0	100.0
8	-20630.0	25270.0	5960.0	11940.0	-12000.0	-3100.0	-5400.0
9	-24579.0	31465.0	-2645.0	20555.0	-15150.0	1250.0	-8850.0
10	-54751.0	52535.0	21190.0	36745.0	-26050.0	-10600.0	-17050.0

Table 3. Coefficients of response surface functions for every load step (Confining pressure 600kPa)

Load step	a	b_1	b_2	b_3	c_1	c_2	c_3
1	-3733.0	5510.0	1670.0	1090.0	-2600.0	-800.0	-500.0
2	-2702.0	4855.0	1130.0	875.0	-2250.0	-500.0	-250.0
3	-3957.0	7280.0	1170.0	1445.0	-3500.0	-500.0	-350.0
4	-13691.0	19685.0	945.0	9075.0	-9750.0	-250.0	-4050.0
5	-6514.0	19105.0	-2110.0	-1610.0	-9150.0	1100.0	1400.0
6	3683.0	26660.0	-13130.0	-17845.0	-13000.0	6500.0	9550.0
7	-9866.0	42955.0	-9960.0	-10210.0	-21150.0	5000.0	5900.0
8	-12339.0	59555.0	-15075.0	-15865.0	-29650.0	7250.0	8850.0
9	1064.0	47920.0	-26850.0	-19710.0	-23700.0	13000.0	10900.0
10	-61362.0	101415.0	-10325.0	34545.0	-50450.0	4850.0	-15950.0

Table 4. Coefficients of response surface functions for every load step (Confining pressure 1200kPa)

Load step	a	b_1	b_2	b_3	c_1	c_2	c_3
1	457.0	-625.0	835.0	-265.0	550.0	-350.0	150.0
2	-234.0	160.0	1090.0	850.0	300.0	-400.0	-300.0
3	1150.0	-2275.0	620.0	1380.0	1850.0	-100.0	-500.0
4	48694.0	-98960.0	-3070.0	2385.0	52700.0	1800.0	-850.0
5	-3356.0	4500.0	2495.0	1905.0	-1000.0	-1050.0	-250.0
6	-10869	15845.0	-2075.0	11170.0	-6750.0	1150.0	-4800.0
7	-3229.0	9035.0	4210.0	-4680.0	-3050.0	-1900.0	3600.0
8	29202.0	-5755.0	-17810.0	-30510.0	4050.0	8700.0	16200.0
9	-89748	75030.0	52945.0	53025.0	-36500.0	-25750.0	-24550
10	-94191	126100.0	16225.0	48875.0	-62400.0	-8150.0	-22050

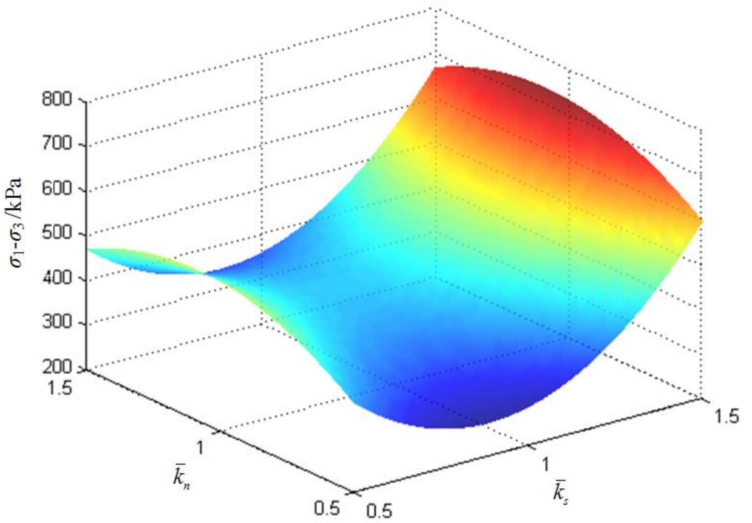

Figure 9. Response surface of deviatoric stress (*f*=1.0, Confining pressure=400kPa)

The objective function of estimating PFC model parameters for rockfill materials is defined as Root Mean Square (RMS)

$$\min J = \sqrt{\frac{1}{N}\sum_{k=1}^{N}[s_k(\bar{\mathbf{x}}) - s_k^m]^2} \tag{13}$$

Where J is objective function of parameter inversion, s_k^m is the observed principal stress differences for the-k loading step in triaxial compression tests of rockfill materials, N is the number of loading step. Equation (13) is an optimization problem with non-constrained conditions and can be solved with some optimization algorithms. So, the inverse problem for parameter estimation is transformed into optimization problem and can be solved with BFGS optimization algorithm [Broyden (1970); Andonegi et al. (2011)]. According to observed data in triaxial compression tests of rockfill materials, as shown in Figure 4, and response surface functions, as shown in Table 2, 3, and 4, as well as BFGS optimization algorithm, unknown PFC model parameters of rockfill materials are identified and listed in Table 5.

Table 5. Identified PFC model parameters of rockfill materials

k_n /MN/m	k_s /MN/m	f	σ_c / kPa
86.504	83.224	0.9175	400
128.88	124.45	0.9192	600
144.31	137.12	1.0389	1200

From Table 5, it will be found that the normal stiffness is slightly larger than tangent stiffness and nearly equal to tangent stiffness. Based on identified PFC model parameters of rockfill materials, variations of deviatoric stress versus axial strain in triaxial compression test of rockfill materials under different confining pressure are simulated again. The differences between observed deviatoric stresses and predicted ones are depicted in Figure 10, 11 and 12. From these figures, we can find that predicted values by PFC model agree well with the experimental ones.

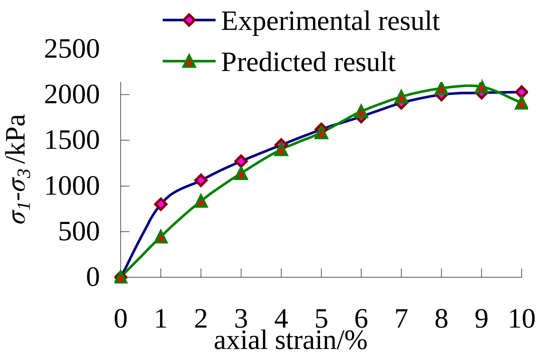

Figure 10. Comparison between experimental values and predicted ones in triaxial compression test (Confining pressure 400 kPa)

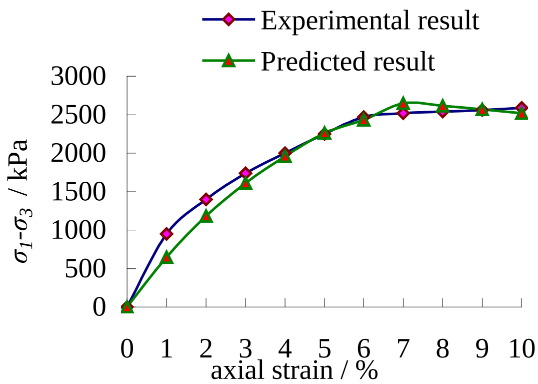

Figure 11. Comparison between experimental values and predicted ones in triaxial compression test (Confining pressure 600 kPa)

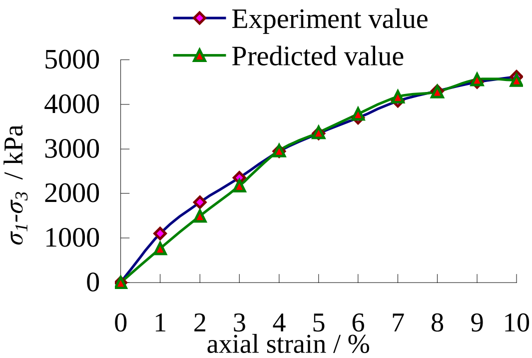

Figure 12. Comparison between experimental values and predicted ones in triaxial compression test (Confining pressure 1200 kPa)

The further investigation facts that the normal stiffness, tangent stiffness and friction coefficient will increase with the increase of confining pressure σ_3, as shown in Table 5 and in Figure 13 and 14. The relations between constitutive model parameters of particles and confining pressures can be expressed as follows

$$k_n = \alpha(\frac{\sigma_3}{P_a})^{\beta} \tag{14}$$

$$k_s = \psi(\frac{\sigma_3}{P_a})^{\zeta} \tag{15}$$

$$f = m(\frac{\sigma_3}{P_a})^{n} \tag{16}$$

Where α, ψ and m are coefficients of empirical equations, β, ζ and n are exponents of empirical equations, P_a is atmosphere pressure, P_a =100kPa. After regression analysis, the coefficients and exponents of empirical equations are determined as follows: α=51.1, β =0.437, ψ =50.5, ζ=0.423, m=0.763, n=0.120.

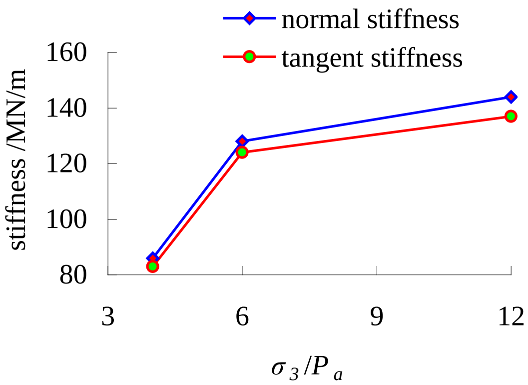

Figure 13. Variation of normal stiffness and tangent stiffness versus confining pressure

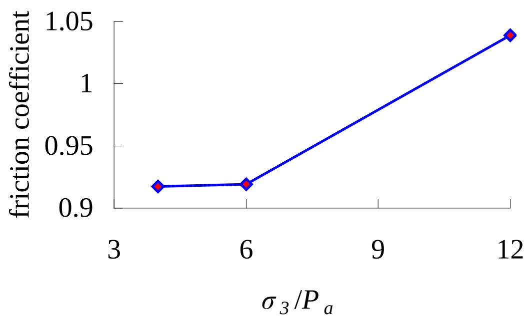

Figure 14. Variation of friction coefficient versus confining pressure

4. Conclusions

1) A new inversion procedure is proposed to determine PFC model parameters of rockfill materials. Based on the response surface method, the relation between unknown PFC model parameters of rockfill materials and deviatoric stress in triaxial compression test is approached. By comparing forecasted stress-strain curves with observed ones, the effectiveness of proposed model parameter inversion procedure is validated by experiments in laboratory.

2) The investigation facts that the normal stiffness is slightly larger than tangent stiffness and nearly equal to tangent stiffness. The normal stiffness, tangent stiffness and friction coefficient will increase with the increase of confining pressure.

3) The nonlinear relations between constitutive model parameters of particles and confining pressures are presented. But the expressions and its coefficients only supply references because the number of samples is not large enough. How to determine pro-fractured mechanical characteristics of rockfill materials should be further investigated in the future.

5. Acknowledgement

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