Estimating micro-property parameters of concrete materials based on macro-experimental data

To cite this article: S J Li *et al* 2019 *IOP Conf. Ser.: Earth Environ. Sci.* **351** 012027

Estimating micro-property parameters of concrete materials based on macro-experimental data

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Abstract. It is very difficult to simulate nonlinear characteristics of concrete materials during fracturing process with continuum mechanics models. Discrete element methods supply for a new way for solving this kind of problems. However, how to precisely determine parameters of micro-constitutive model of concrete materials has become a key problem that affects the development and practical application of discrete element methods. The nonlinear mapping relation between deformation data of concrete specimen and parameters of micro-constitutive model of concrete materials is bridged by response surface function. Based on macro experimental data and response surface function, parameters of micro-constitutive model of concrete materials are determined by using optimization algorithm. The investigation result validates that the forecasted stress-strain curve for concrete specimen agrees well with observed one. The parameter inversion of micro-constitutive model for concrete materials can supply for foundations for precisely numerical simulation of discrete element methods.

1. Introduction
Particle flow code (PFC) software has widely used to simulate rock fragmentation process, crack propagation in rock, soil-tool interaction, and slope stability analysis. How to precisely determine micro-constitutive model of concrete materials is very important for simulating crack propagation in concrete materials. Mak proposed a numerical procedure based on PFC software to estimate model parameters of cohesive soils. In the micro-parameters of soil model, the shear strength between particles was directly chosen as soil cohesion in macro shear test. The normal strength was determined by internal fraction angle and cohesion in macro shear test [1]. This assumption is suspicious. Potyondy proposed a bonded-particle model for rock. The micro-properties consisted of stiffness and strength parameters for the particles and the bonds. This research established foundation to simulate cohesive materials fracture process and provide conceptual model to investigate the micro-mechanism of complex macro-behaviour of rock or concrete fracturing process [2]. Ucgul developed an approach to determine contact model and parameters for a cohesionless soil from angle of repose and penetration tests, matching the simulation results to test results [3]. The inversion method cannot be available to concrete materials with cohesion. Asaf used Nelder-Mead algorithm of optimization to estimate soil model parameters by penetration tests. The proposed method was verified experimentally and numerically [4]. The inversion procedure provided a practical way to determine soil micro-parameters by combining numerically simulation and model experiments. Azevedo presented an

approach to model aggregate as a deformable group of particles. The inter-particle contacts were assumed as brittle or follow a given bilinear softening curve. The proposed softening contact model can agree well with experimental curves [5]. Gu developed rigid-body-spring concrete model by considering the contact between elements after the failure of the springs. This concrete model included coarse aggregates, the mortar and their interface. The micro-model can simulate the random distribution of coarse aggregate [6]. In order to estimate model parameters, triaxial compression experiments of rockfill materials were performed by Li [7]. Based on a genetic algorithm, the constitutive model parameters of the rockfill material were determined from the triaxial compression experimental data. Based on triaxial compression experiment data and optimization algorithm, the model parameters of rockfill materials are estimated. James proposed a micro model to couple ductile damage models with Beremin-like failure probability, and predicted the fracture toughness in a large part of the transition region [8]. Based on response surface method and PFC software, micro-parameter of rockfill materials were estimated by comparing the difference between simulated deformation curves and test curves of rockfill materials. By using response surface method, the nonlinear mapping relation between deformation data of rockfill materials and parameters of micro-constitutive model of rockfill materials was established [9]. The proposed response surface method is utilized to estimate concrete material parameters. Coetzee presented a procedure to calibrate discrete element parameters for simulating silo discharge and bucket filling. The investigation showed that shear test results are dependent on both the particle friction coefficient and the particle stiffness. The calibration procedure was validated by numerical simulation [10]. The aim of the paper is to propose a procedure to determine parameters of micro-constitutive model of concrete materials based on macro-experimental data of uni-axial compressive test of concrete specimens. The response surface method is applied to bridge relationship between macro-deformation data of concrete specimen and parameters of micro-constitutive model of concrete materials.

2. Micro-property parameters of parallel-bond behavior of concrete materials

Contact behavior of unbonded particle material can be represented as three parameters: normal contact stiffness k_n, tangent contact stiffness k_s, and fraction coefficient f, as shown in Figure 1.

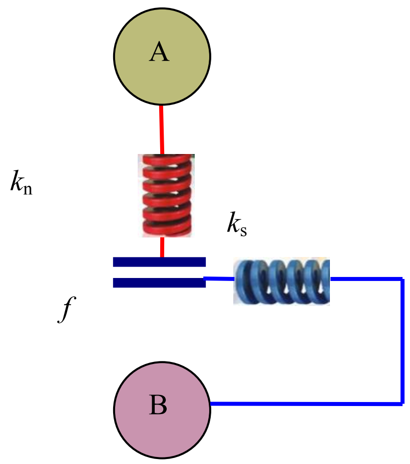

Figure 1. Unbonded contact model between tow particles in PFC.

Contact behavior of parallel-bounded material can be represented by above three parameters and following five parameters: normal strength σ_t between two particles jointed by a contact bond, shear strength τ_s of contact bond, normal contact stiffness k_{nb} of contact bond, tangent contact stiffness k_{sb} of contact bond and bond radius R_b for bond materials, as shown in Figure 2.

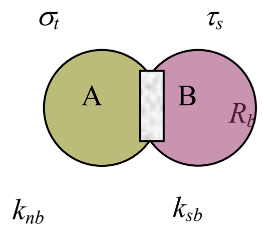

Figure 2. Parallel-bond model with a cylindrical bond of cementitious material between tow particles in PFC.

The estimated micro-property parameters of parallel-bond behavior of concrete materials can be expressed as a vector x:

$$x = \{k_n, k_s, f, \sigma_t, \tau_s, k_{nb}, R_b, k_{sb}\}^T \tag{1}$$

where k_n is normal contact stiffness of particles, k_s is tangent contact stiffness of particles, and f is fraction coefficient between particles. The contact normal stiffness of particles can be expressed by contact Young's modulus E_c

$$k_n = \frac{AE_c}{L} \tag{2}$$

where L is beam length, $L=RA+RB$, A is beam cross-sectional area [2]. The parallel-bonded normal stiffness can be expressed by contact Young's modulus E_{cb} of bond materials [2]:

$$k_{nb} = \frac{E_{cb}}{L} \tag{3}$$

In order to simplify constitutive model of concrete material, proving the contact Young's modulus of bond materials E_{cb} is equal to contact Young's modulus of particles. Another hypothesis is described as:

$$n = \frac{k_n}{k_s} = \frac{k_{nb}}{k_{sb}} \tag{4}$$

$$R_b = \min(R_A, R_B) \tag{5}$$

So, the estimated micro-property parameters of parallel-bond behavior of concrete materials can be rewritten as follows:

$$x = \{E_c, n, f, \sigma_t, \tau_s\}^T \tag{6}$$

If the model parameters are known, the deformation property of concrete material can be numerically simulated. Numerical model for simulating uni-axial compressive test of concrete material is shown in Figure 3. Based on some reference documents, initial estimated micro-property parameters of concrete materials are determined as Table 1.

Table 1. Initial estimated micro-property parameters of concrete materials.

Micro-parameters	E_c（GPa）	$n=k_n / k_s$	f	σ_t（MPa）	τ_s（MPa）
Grade C60	30.0	1.0	1.0	30.0	30.0

Figure 3. Numerical model in micro scale for simulating uni-axial compressive test of concrete material.

3. Response surface methods for estimating micro-properties parameters of concrete materials

Response surface method is used to bridge relationship between macro-deformation data of concrete specimen and parameters of micro-constitutive model of concrete materials. Response surface function for vertical strain of concrete specimen versus micro-parameters can be expressed as:

$$\varepsilon_k(x) = a + \sum_{i=1}^{5} b_i x_i + \sum_{i=1}^{5} c_i x_i^2 \tag{7}$$

where ε_k denotes vertical strain in the *kth* loading step for uni-axial compressive test, it is the function of estimated micro-parameters of concrete materials, a、b_i and c_i denotes undetermined coefficients of polynomial function, x denotes estimated micro-parameters vector. Taking in the first loading step in uni-axial compressive test as an example, the equation (7) can be extended as follows:

$$\varepsilon_1^1(\mathbf{x}) = \varepsilon(k_n, f, \sigma_t, \tau_s, k_s) \tag{8}$$

$$\varepsilon_1^2(\mathbf{x}) = \varepsilon(k_n + \Delta k_n, f, \sigma_t, \tau_s, k_s) \tag{9}$$

$$\varepsilon_1^3(\mathbf{x}) = \varepsilon(k_n - \Delta k_n, f, \sigma_t, \tau_s, k_s) \tag{10}$$

$$\varepsilon_1^4(\mathbf{x}) = \varepsilon(k_n, f + \Delta f, \sigma_t, \tau_s, k_s) \tag{11}$$

$$\varepsilon_1^5(\mathbf{x}) = \varepsilon(k_n, f\text{-}\Delta f, \sigma_t, \tau_s, k_s) \tag{12}$$

$$\varepsilon_1^6(\mathbf{x}) = \varepsilon(k_n, f, \sigma_t + \Delta\sigma_t, \tau_s, k_s) \tag{13}$$

$$\varepsilon_1^7(\mathbf{x}) = \varepsilon(k_n, f, \sigma_t - \Delta\sigma_t, \tau_s, k_s) \tag{14}$$

$$\varepsilon_1^8(\mathbf{x}) = \varepsilon(k_n, f, \sigma_t, \tau_s + \Delta\tau_s, k_s) \tag{15}$$

$$\varepsilon_1^9(\mathbf{x}) = \varepsilon(k_n, f, \sigma_t, \tau_s - \Delta\tau_s, k_s) \tag{16}$$

$$\varepsilon_1^{10}(\mathbf{x}) = \varepsilon(k_n, f, \sigma_t, \tau_s, k_s + \Delta k_s) \tag{17}$$

$$\varepsilon_1^{11}(\mathbf{x}) = \varepsilon(k_n, f, \sigma_t, \tau_s, k_s - \Delta k_s) \tag{18}$$

where $\varepsilon_1^j(x)$ is axial strain of concrete specimen in first loading step computed by PFC while the micro-parameters of concrete are chosen as right hand item in equations from 8 to 18, Δk_n denotes increment of normal stiffness of two particles, other parameter increments are defined as above. Left hand item in Equations from 8 to 18 can be numerically calculated by PFC software while the initial model parameters are determined in Table 1. There are 11 undetermined coefficients in polynomial function in equation 7, and there are equations from 8 to 18. So, the coefficients of polynomial function can be easily determined. For other loading steps, the coefficients of polynomial function can be determined as above-mentioned method. Experimental specimen of concrete material in uni-axial compressive test is shown in Figure 4. Observed macro-experimental data for uni-axial compressive test for different concrete grade are shown in Figure 5. These macro-experimental data are foundations for estimating micro-property parameters of concrete materials.

Figure 4. Experimental specimen of concrete material in uni-axial compressive test.

As shown in Figure 4, the uni-axial compressive tests for concrete specimen are performed. The size of concrete specimen is 150mm*150mm*300m. The sand coarse aggregate ratio of mixed concrete is 32%. Water cement ratio is 0.27-0.28. The one cubic meter of concrete mix requires ingredients as: cement 430kg, fly ash 70kg, breeze 50kg, sand 680kg, pebble 1040kg, water 150kg. The maximum and minimum size of aggregate is 40mm and 0.3mm, respectively. The axial force, vertical displacement, and axial strain and horizontal strain are recorded at every loading step during compressive tests, as shown in Figure 5.

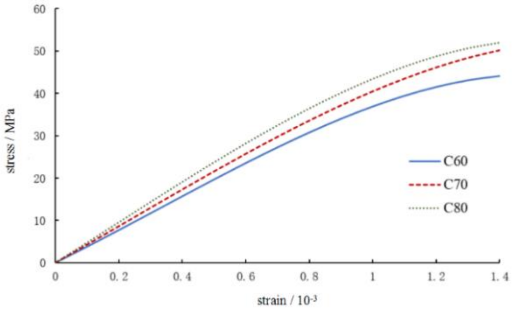

Figure 5. Observed macro-experimental data for uni-axial compressive test for different concrete grade.

4. Estimating micro-properties parameters of concrete materials by using response surface method

Before estimating micro-properties parameters of concrete materials, sensitivity analysis is performed. Influence of shear strength τ_s of bond materials on deformability in macro-experimental test is shown in Figure 6. It can be observed from Figure 6 that the compressive strength of concrete specimen increases with increasing shear strengthτs of bond materials.

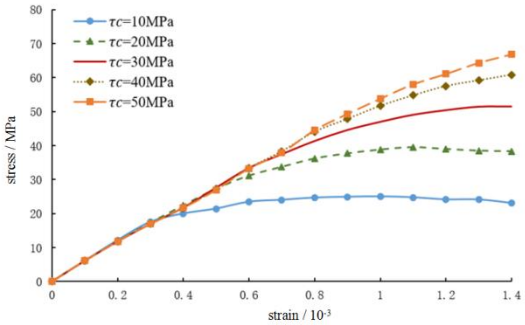

Figure 6. Influence of shear strength of bond materials on deformability in macro-experimental test model simulated by PFC

In order to estimate micro-parameters of concrete materials, the objective function of parameter inversion is defined as:

$$\min J = \sum_{k=1}^{N}[\varepsilon_k(x) - \varepsilon_k^m]^2 \quad (19)$$

where J is objective function of parameters inversion, ε_k^m is observed axial strain of concrete specimen in *kth* loading step in uni-axial compressive test, N is loading steps, in this research N=14. The parameter inversion problem is changed into optimization problem. DFP (Davidon-Fletcher-Powell) optimization algorithm or BFGS (Broyden-Fletcher-Goldfarb-Shanno) optimization algorithm in MATLAB will be used to solve optimization problem after initial micro-parameters of concrete materials are determined and response surface functions are calculated based on PFC software. Estimated micro-property parameters of concrete materials are listed in Table 2.

Table 2. Estimated micro-property parameters of concrete materials.

Micro-parameters	E_c (GPa)	$n=k_n/k_s$	f	σ_t (Mpa)	τ_s (Mpa)
Grade C60	21.83	1.11	0.99	37.12	25.27
Grade C70	23.10	1.15	1.11	39.25	26.07
Grade C80	24.89	1.11	1.15	40.62	26.39

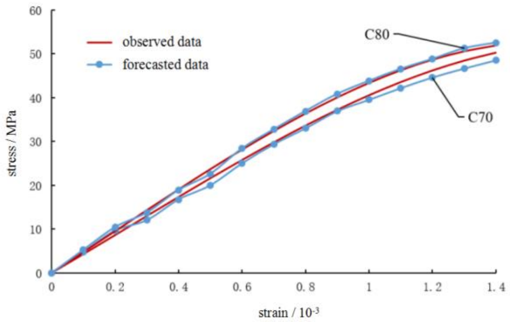

Figure 7. Comparison between observed data and forecasted ones (concrete Grade C70 and C80).

It can be observed from Figure 7 that forecasted stress-strain curves agree well with experimental curves and effectiveness of proposed estimation procedure is validated.

5. Conclusion

The investigation shows that the shear strength τ_s of contact bond (25.27MPa) is much greater than shear strength of concrete macro-specimen (5.6MPa). So, the assumption proposed by Mak [1], in which the shear strength τ_s of contact bond in micro-model is equal to shear strength of concrete macro-specimen, is incorrect or at least inaccurate. The normal strength between two particles jointed by a contact bond and shear strength of contact bond are different from tensile strength and shear strength in macro-test.

Estimating micro-parameters of concrete material based on macro-experimental data is a new idea. The forecasted stress-strain curve for concrete specimen agrees well with observed one. The correctness of proposed inversion procedure is validated by experimental results. The contact normal stiffness between two particles is approximately equal to tangent contact stiffness between two particles. This conclusion agrees with suggestions by Cundall [11].

The fraction coefficient between two contact particles is approximately equal to 1.0. The micro-parameters of concrete material increase slightly with increasing of concrete grade. The internal fraction angle of C60 concrete is approximately 63 degree. The fraction coefficient of C60 concrete in macro-dimension is 1.92. So, the fraction coefficient of concrete materials in micro-dimension is different from the fraction coefficient in macro-dimension.

The tensile test and direct shear test for concrete materials should be added in future investigations in order to cancel some proposed hypothesis and estimate more micro-parameters and accurately forecast deformation and strength properties of concrete materials.

Acknowledgements
This work was supported by the National Program on Key Basic Research Project of China (973 Program) (2015CB057804).

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