Study on Identification of Material Model Parameters from Compact Tension Test on Concrete Specimens

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Abstract. Identification of a concrete material model parameters using optimization is based on a calculation of a difference between experimentally measured and numerically obtained data. Measure of the difference can be formulated via root mean squared error that is often used for determination of accuracy of a mathematical model in the field of meteorology or demography. The quality of the identified parameters is, however, determined not only by right choice of an objective function but also by the source experimental data. One of the possible way is to use load-displacement curves from three-point bending tests that were performed on concrete specimens. This option shows the significance of modulus of elasticity, tensile strength and specific fracture energy. Another possible option is to use experimental data from compact tension test. It is clear that the response in the second type of test is also dependent on the above mentioned material parameters. The question is whether the parameters identified within three-point bending test and within compact tension test will reach the same values. The presented article brings the numerical study of inverse identification of material model parameters from experimental data measured during compact tension tests. The article also presents utilization of the modified sensitivity analysis that calculates the sensitivity of the material model parameters for different parts of loading curve. The main goal of the article is to describe the process of inverse identification of parameters for plasticity-based material model of concrete and prepare data for future comparison with identified values of the material model parameters from different type of fracture tests.

1. Introduction
Detailed analysis of structure response is enabled by utilization of geometrical [1, 2] and material nonlinearity [3, 4] within numerical simulation. This development is supported by the potential of current information technologies, and by results achieved within theoretical research into nonlinear material models. The analysis, however, suffers from complexity of material models that are based on assumptions of different theories. The combination of different theoretical approaches particularly in case of concrete material models leads to situation where the values of material model parameters are not known in advance.

Within nonlinear material models of concrete, it is possible to identify several branches of development. One of such branches exploits the postulates of linear and nonlinear fracture mechanics, described in detail by the authors of reference [5], and is aptly complemented with another category, which has grown upon the assumptions of plasticity theory. A well-conceived historical survey of the material models is proposed within relevant papers by Cickele et al. [6] and Grassl et al., [7]; both
these articles, however, also suggest that using pure plasticity theory to describe the behaviour of concrete structures does not constitute a satisfactory procedure, mainly due to the decreasing material stiffness caused by the formation and development of cracks. This view then inspired the development of damage theory. The results obtained from the research in this field nevertheless indicate that the use of the theory as a sole tool is again not entirely optimal, primarily owing to the inability of the derived material models to capture emerging irreversible deformations and inelastic volume changes of concrete [7]. In the context of developmental categories within the modelling of nonlinear behaviour in concrete, we can point further to the SPH methods [8,9] and the widely favoured XFEM (extended finite element method) [10]. The above-mentioned drawbacks of inherent with some of the theories are suitably eliminated via combining the tools into a single concept, observing their mutual complementarity. Currently, we can thus utilize material models of concrete which join together plasticity and damage theories or combine plasticity theory with the theoretical fundamentals of nonlinear fracture mechanics. An example of the latter approach consists in multiPlas, a database of elastoplastic material models [11] to facilitate nonlinear material computation via the finite element method in ANSYS [12].

The correct application of the discussed models rests upon a relatively broad set of input parameters of the given material model. As it was mentioned above, the values of such parameters are not known in advance; however, the problem can be solved through a simple fracture experiment with subsequent inverse identification of the parameters from the measured data. Within inverse identification, we can employ methods exploiting the training of artificial neural networks [13] or, alternatively, an optimization algorithm [14, 15]. The inverse identification procedure with optimization is based on the effort to reduce the difference between a measured loading curve and one produced by the numerical simulation of a fracture test performed on a computing system. The reference experimental data can be represented by load-displacement curves from three-point bending test which were used by authors in [16,17] but also by points from compact tension (CT) test or wedge splitting test (WST). The two last mentioned experiments are such substitution of the direct tensile test and they produce \( L\text{-CMOD} \) curves where the opening of the notch is measured.

The presented article brings the study on inverse identification of material parameters of Menetrey-Willam material model of concrete from multiPlas database [11]. The paper contains a description of the computational model of the CT test, a description of the performed sensitivity analysis, and description of the process of identification of significant material model parameters. The main goal of the article is to show problems that occurs when this type of fracture test is numerically simulated and summarize conclusions for future comparison of results of identification that are going to be performed with data from three-point bending test and CT test on the specimens from the same concrete. This comparison will show, whether the implementation of Menetrey-Willam material model is correct in the multiPlas database.

2. Description of input data and fracture experiment

In order to perform the inverse identification of material parameters of the given constitutive law, we chose one \( L\text{-CMOD} \) curve associated with the set of compact tension (CT) test published by Wittman et al. [18]. The CT test is a different testing method to the three-point bending test which was suggested in the RILEM [19] for determination of fracture energy \( G_f \). The configuration of the CT test and dimension of the chosen specimen are shown in figure 1.
Figure 1. Configuration of the CT fracture test and dimensions of the specimen (adopted from [18])

The authors of the cited article had performed test on fourteen CT specimens with different dimensions, concrete composition and loading rate [18]. However, we adopted only one experimental mean $L$-$CMOD$ curve that were measured on the largest CT specimen. The form of the chosen curve is shown in figure 2.

Figure 2. Reference experimental $L$-$CMOD$ curve (adopted from [18])

3. Computational model
The computational model of the analysed fracture experiment was prepared in the classic environment of the ANSYS 15.0 computational system with utilization of the Menetrey-Willam material model for concrete from external database of nonlinear material models called multiPlas. The sensitivity analysis and inverse identification itself were performed in ANSYS Workbench 15.0 where robust optimization algorithms are implemented at present.
3.1. Geometry of the computational model
The geometry of the computational model of the CT specimen was, in all of the above-mentioned dimensions, covered with mesh of four node planar finite elements (PLANE182). The task was solved as a plane stress problem, with the thickness of 120 mm assigned to all elements of the model. The task had been simplified from a 3D problem to a 2D plane stress one in order to reduce the computational time to a single numerical simulation. The notch in the test sample was modeled using two lines having a common node at the top of the notch. The load in the model had been entered as horizontal deformation $d_{\text{max}}$ exhibiting the magnitude of 0.00062 m.

The deformation load was prescribed at the central node of the steel cylinders that were also modeled with planar elements (PLANE182). This modeling technique required the placement of line elements of the contact pair CONTA171 and TARGE169. Contact between the concrete specimen and steel cylinders, using the Lagrange contact algorithm, was modeled from both sides. This means that contact (CONTA171) and target (TARGE169) elements were modeled both on the outer line of the hole in the CT specimen and on the inner line of the steel cylinder. The form of the above described geometry of the computational model is shown in figure 3.

![Computational model of CT specimen](image)

3.2. Material model
The applied material model, Menétry-Willam, belongs to the group of nonlinear material models of concrete that cannot capture the effect exerted by the rate of deformation on the stress condition. In these models, irreversible deformations occur when the preset plasticity criterion is achieved, and the total deformation vector $\varepsilon_{\text{tot}}$ is assumed to decompose into an elastic $\varepsilon_{\text{el}}$ and a plastic $\varepsilon_{\text{pl}}$ part [20].

The criterion of the generation of plastic deformations is given by the prescribed yield surface function. The selected material model, Menétry-Willam [21], exploits the Willam-Warnke yield surface [22], which, unlike the Drucker-Prager one, embodies the function of not only the first and the second but also the third invariant of the deviatoric stress tensor (referred to as lode angle). Such adjustment enables us to refine the angles of the deviatoric sections of the yield surface, whose distance from the hydrostatic axis in Haigh–Westergaard stress space is moreover not constant.

From the point of view of using the finite element method, the selected material model utilizes the smeared cracks approach [23]. Further, the given problem was solved employing the version with the softening function based on the dissipation of the specific fracture energy $G_{\text{fs}}$, which thus acts as one of the parameters being sought. With respect to the need of eliminating the negative dependence of the solution on the size of the finite element mesh, the Menétry-Willam nonlinear model uses Bazant’s
crack band concept [24]. To facilitate the corresponding nonlinear behavior of the model, we had to redefine 12 parameters in total; these are briefly characterized in Table 1 below.

**Table 1. A definition of the Menétrey-Willam material model parameters**

| Parameter | Unit | Description |
|-----------|------|-------------|
| $E$       | [Pa] | Young’s modulus of elasticity |
| $v$       | [-]  | Poisson’s ratio |
| $f_c$     | [Pa] | Uniaxial compression strength |
| $f_t$     | [Pa] | Uniaxial tension strength |
| $k$       | [-]  | Ratio between biaxial compressive strength and uniaxial compressive strength |
| $\psi$    | [°]  | Dilatancy angle (friction angle) |
| $\varepsilon_m$ | [-] | Plastic strain corresponding to the maximum load |
| $G_{fc}$  | [Nm/m²] | Specific fracture energy in compression |
| $\Omega_{ei}$ | [-] | Relative stress level at the start of nonlinear hardening in compression |
| $\Omega_{cr}$ | [-] | Residual relative stress level in compression |
| $G_{ft}$  | [Nm/m²] | Specific fracture energy in tension |
| $\Omega_{tr}$ | [-] | Residual relative stress level in tension |

4. Problem solution

The solution of the problem was divided into two stages. First, the sensitivity analysis was performed. The main purpose of the sensitivity analysis was to find influence of the material model parameters on the value of the objective function. Second, the inverse identification of the material model parameters values using optimization method was conducted.

4.1. Sensitivity analysis

Sensitivity analysis is basically a task which seeks the level to which output data uncertainties are influenced by the variability of input data [25]. As a result, these methods are very suitable as optimization pre-processing tools, though a certain disadvantage of such methods is their high requirements regarding the number of simulations required. Before the sensitivity analysis itself, several pilot simulations were performed. The purpose of these simulations was to find delimiting curves. These curves were used for the delimitation of the area of the covered space of input values with random realizations using the LHS method. During the search for these curves, which was completely empirical and based on the experience of the authors, two basic sets of material model parameters were created. With the help of these sets, the range of individual parameters could consequently be limited, which resulted in the significant simplification and primarily the acceleration of the whole inverse identification process. Another positive aspect of this procedure was the verification of the convergence of the numerical solution for the limit values of parameters, and thus the creation of the prerequisite for smooth convergence within the design intervals of the sought parameters. The form of the boundary curves and their position with regards to the reference L-CMOD curve is documented in figure 4.

The first step of the performed sensitivity analysis was to select the correct output parameter (i.e. the objective function). In accordance with Hyndman et al. [26], we chose the Root-Mean-Squared Error (RMSE) measure; this is often used for the calculation of the difference between the values generated by a mathematical model and those that are observed.
Figure 4. Reference $L$-CMOD curve with delimiting curves for sensitivity analysis

Such a measure is therefore utilized in meteorology, economics, and demography. The RMSE measure is expressed as follows:

$$
RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (y_i^* - y_i)^2},
$$

where $y_i^*$ is the value of the force calculated within the framework of the numerical simulation, and $y_i$ denotes the value of the force gained from the experimental $L$-CMOD curve. However, the direct calculation of the RMSE measure value was complicated by different positions of the points of the numerical and experimental $L$-CMOD curves; this difference had been caused by bisections that occurred during nonlinear solution. It was then necessary to map the points of the numerical $L$-CMOD curve according to the points of the experimental curve, and this process was performed via linear interpolation.

The sought sensitivity was expressed by calculating the Spearman rank-order coefficient of correlation $r_s$. The calculation of the correlation coefficient was conducted through the use of the programmed Python script. Given that the material parameters and the RMSE measure are real numbers, the value of the Spearman correlation coefficient was calculated using the formula:

$$
r_s = 1 - \frac{6 \sum_{i=1}^{m} \delta_i^2}{m(m^2 - 1)},
$$

where

$$
\delta_i = \text{rank}(X_i) - \text{rank}(Y_i)
$$

is the difference between the ranks of each observation, and $m$ denotes the number of observations.
In order to reduce requirements of the high number of simulation, the calculation of the objective function (1) was performed not only over the whole \( L-CMOD \) curve but also on five parts of the curve. This modification led to reduction of the full design vector to the form:

\[
X_{\text{red}} = \begin{bmatrix} E \\ f_t \\ G_{f_r} \end{bmatrix}
\]

The stated results of the sensitivity analysis performed with 85 simulations are documented by 5 bar charts in figure 5.

Figure 5. Sensitivity bar charts (a) RMSE 1 – (e) RMSE 5
4.2. Identification of material model parameters using optimization

The inverse identification of the values of the material model parameters was performed with respect to results of the previous sensitivity analysis. It means that only values of three significant parameters (i.e. Young’s modulus of elasticity $E$, uniaxial tensile strength $f_t$ and specific fracture energy in tension $G_{ft}$) were identified using genetic optimization algorithm MOGA in ANSYS Workbench. The optimization task was defined as minimization of the objective function defined as RMSE in equation (1). The optimization procedure was set up to create 50 initial realizations of design vector with 10 realizations in each generation. The maximum number generations were limited to 20.

5. Results

The resultant set of the sought material model parameters was achieved in 93rd realization of the design vector with final RMSE value of 549.39. The relatively good agreement between experimental and final numerical $L$-$CMOD$ curve is clearly visible in figure 6.

![Figure 6. Comparison of the reference and the identified $L$-$CMOD$ curve](image)

The values of the identified Young’s modulus of elasticity $E$, uniaxial tensile strength $f_t$ and specific fracture energy $G_{ft}$ are summarized in table 2 below.

| Parameter | Unit       | Value       |
|-----------|------------|-------------|
| $E$       | [Pa]       | $32.901\cdot10^9$ |
| $f_t$     | [Pa]       | $2.005\cdot10^6$  |
| $G_{ft}$  | [Nm/m²]   | $68.206$   |

The identified values of modulus of elasticity $E$ and uniaxial tensile strength $f_t$ cannot be compared with cited publication because the authors of the article performed several numerical simulations with different setup of the tensile strength and fracture energy. On the other hand, the identified value of the specific fracture energy $G_{ft}$ is significantly lower than value presented by Wittmann et al. [18]. The difference exceeded 56.83%.
6. Conclusions
The above presented results show that is possible to simulate nonlinear response of concrete CT specimen during CT test with utilization of Menetrey-Willam material model. With respect to the achieved results it can be said that the identification of unknown values of material parameters via optimization with incorporation of sensitivity analysis can be used as a useful tool for searching values of parameters that appeared within complex constitutive laws. The stated difference of the specific fracture energy value $G_{ft}$ could be caused by different implementation of the concept of the specific fracture energy in multilPlas database which will be subjected to further research. With respect to the conclusions of the cited article [18] the influence of the dimensions of the CT specimens to values of the parameters of the selected material model will be also examined.

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