Nonlinear numerical simulation of a fracture test with use of optimization for identification of material parameters

Filip Hokes, Jiri Kala, and Ondrej Krnavek

***Abstract*—**The application of a nonlinear description of construction material behaviour in numerical simulations represents a step forward in enabling mathematical modeling methods to ever more closely describe the real actions of structures. This statement is also valid in the case of the numerical modeling of fracture experiments, but in both cases this modeling is complicated by the existence of unknown material parameters for the nonlinear material model. However, fracture experiments provide the opportunity to identify unknown parameters from data that are measured during the performance of such experiments. The submitted article deals with the numerical simulation of a three-point bending test carried out on a concrete specimen. It describes the process by which the inverse identification of material parameters takes place via optimization. The inverse analysis was based on the utilization of a load-displacement curve measured during the experiment. The main aim of the article is to present a method describing the inverse identification of parameters from the simulation of a fracture experiment which can then be used in the performance of comprehensive nonlinear simulations of the behaviour of structural details and whole structures manufactured from concrete.

***Keywords*—**Concrete, evolution strategy, fracture test, genetic algorithm, nonlinear material model, sensitivity.

I. Introduction

THE numerical solution of problems in the area of structural design has been very popular for many years. This popularity is a result of both the already very good existing knowledge of numerical methods of mathematical modelling and, among other things, the fact that the numerical simulation of certain complex and atypical structural elements in computational systems such as ANSYS [1] or LS-Dyna [2] is significantly cheaper than the experimental testing of real specimens [3], [4]. Both approaches may also be advantageously combined as was shown by Kala *et al.* [5], Kala and Husek [6], Kral *et al.* [7] and Kralik *et al.* [8]. Despite the level of development of current computational tools, efforts are constantly underway to improve them still further, which is most true of all for the area of nonlinear mechanics.

Research into the description of the nonlinear behaviour of materials and the testing of the usability of derived constitutive relationships in the calculations needed for specific civil engineering and mechanical engineering tasks is of high importance. With the correct use of an exact model, and when the given prerequisites are fulfilled, the closer approximation of a simulation to the real behaviour of a structure can be achieved with numerical calculations. One result of such an approximation may be the design of still more economical and safer buildings.

One of the materials whose wide implementation in construction requires the constant improvement of design methods is concrete. For this reason it is essential to understand the nonlinear behaviour of concrete. However, the construction of a correct constitutive relationship which is able to express this nonlinear behaviour for various types of loading appears to be problematic [9]. One of the basic problems which arise when formulating a material model for concrete is the different responses of the material to tensile and compressive load [10]. For this reason, several approaches are used for the mathematical description of the behaviour of concrete. One of these approaches involves the use of theory of plasticity. Applications of theory of plasticity to the description of the behaviour of plain concrete can be found in the work of authors Chen and Chen [11], Willam and Warnke [12], Bazant [13], Dragon and Mroz [14], Schreyer [15], Chen and Buykozturk [16], Onate [17], Pramono and Willam [18], Etse and Willam [19], Menetrey and Willam [20], and Grassl [21]. The material models presented in these publications use standard theory of plasticity for the description of the behaviour of concrete. However, this is not sufficient due to the gradual decrease in the stiffness of concrete due to the occurrence of cracks [9]. This problem can be removed when damage theory is used, i.e. by using an adequate damage model. However, as Grassl claims [22], independent damage models are not sufficient when the description of irreversible deformations and the inelastic volumetric expansion of

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concrete is required. Applications of damage models to the description of the behaviour of concrete can also be found in publications by the authors Loland [23], Ortiz and Popov [24], Krajcinovic [25], Resende and Martin [26], Simo and Ju [27], [28], and Lubarda [29]. Despite the above-mentioned limitations of both approaches, there are advantages to using both of them in mutual combination, and they can be combined further with other approaches formulated within the framework of nonlinear fracture mechanics. The first group of combined models is, according to Cicekli [9], based on stress-based plasticity formulated in the effective stress space; see [30]–[33]. Effective stress is defined in this group of models as the average micro-scale stress affecting an undamaged material between defects. The second group of models is based on stress-based plasticity formulated in the nominal (damaged) stress space [9]; see [34]–[39]. For this group of models, the nominal stress is defined as macro-scale stress affecting both the damaged and the undamaged part of the material [9].

At present, other important trends in the area of nonlinear modelling of the behaviour of concrete can be identified. One of these trends consists in the expansion of the standard finite element method (FEM) into what is known as the extended finite element method (XFEM), in which the need for remeshing is removed. More detailed information can be found in the publications Belytschko and Black [40], Moes *et al.* [41], and Daux *et al.* [42]. Another important trend in the given field is based on the use of the discrete element method, descriptions of which are contained in the works of Cundall [43], and Ghaboussi and Barbosa [44]. This method, however, moves away from continuum theory and uses other prerequisites than plasticity and damage theories. Neither this approach nor the XFEM method is the subject of interest of the group of authors of this contribution. Based on the information provided by the above-mentioned literature in the field of constitutive relationships which combine several approaches within the framework of one material model, the multiPlas [45] database of elasto-plastic materials was developed for application in nonlinear simulations in the ANSYS system environment.

However, the use of this and similar tools results in a problem in real life in the form of the large amount of parameters which need to be known for the selected material model before the launch of the numerical simulation itself. Unfortunately, not all data regarding these parameters, which can be both mechanico-physical and fracture-mechanical in nature, may be available in advance.

In the above-mentioned situation it is possible to make advantageous use of experimentally obtained load-displacement curves measured during the testing of test specimens fabricated from selected materials and reverse identify needed parameters with the aid of inverse identification. Basic information about the issues involved in inverse identification is provided in the work of authors Gavrus *et al.* [46] and Planas *et al.* [47].

The inverse identification process is currently executed by exercising artificial neural networks, or with the help of optimization algorithms implemented in academic or commercial optimization software tools. The form of inverse identification based on the exercise of artificial neural networks was described in publications by the authors Fairbairn *et al.* [48], and Novak and Lehky [49]. The second form of inverse identification, which uses optimization algorithms, was described e.g. in the work of Braasch and Estrin [50], and Vaz *et al.* [51]. General information about use of design optimization techniques in the area of structural engineering problems was published by Fedorik *et al.* [52]. Another way of utilization of optimization techniques for probabilistic design and analysis of load-carrying capacity of structures were published by Krejsa *et al*. [53].

In the case of inverse identification using optimization, the optimization task can be defined as the minimization of the difference between the experimental load-displacement curve and a curve obtained as the output of a numerical simulation in the selected computational system. In such a task, the design vector is created by previously unknown parameters of the nonlinear material model while the delimiting conditions are derived from the prerequisites from which the used material model was derived, or from the requirement for the smooth convergence of the solution.

II. Definition of the Problem

The inverse identification of parameters for the material model from the multiPlas library was performed on a load-displacement curve obtained from the results of a three-point bending test performed on a notched concrete beam, which were published by Strauss *et al.* [54]. The dimensions of the beam were 360 x 120 x 58 mm. In order to achieve savings with regard to the computation time needed for the nonlinear simulation, the complexity of the plane stress task was reduced from 3D to 2D. The appearance of the test specimen is depicted in Fig. 1

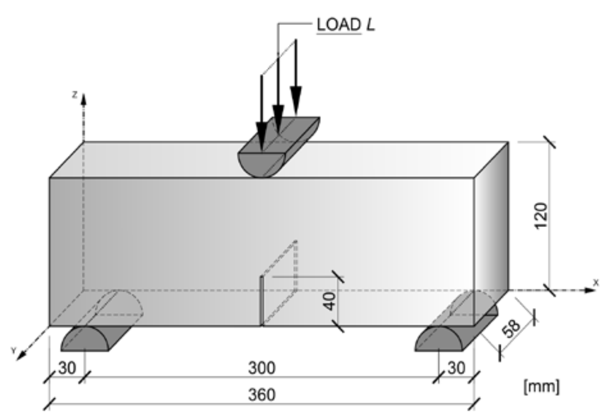

Fig. 1 Scheme of testing configuration

With regard to the simplification mentioned above, boundary conditions were also simplified. In real experiments, support and the application of load are both provided using steel cylinders. When the numerical simulations were carried out, zero vertical displacements were prescribed at the supports. The application of load was also realized in the form of vertical displacement, in order to maintain solvability and obtain the convergence of the solution, horizontal displacement was prevented at the load input location.

A. Analysis of the input data

The publication by Strauss *et al.* [54] presented tests on four sets of concrete specimens of strength class C25/30, as stipulated in [55]. Within these four sets, concrete mixtures with slump values of F45 and F70 were combined and then tested at the age of 28 and 170 days. Each set was composed of 5 test specimens. The concrete specimens were subjected to three-point bending tests, the output of which was a diagram of the dependence of loading force L (measured on a testing machine) and displacement d (measured on the test specimen at midspan).

For the purposes of the presented article, only one load-displacement curve was chosen for one of the test specimens with a slump value of F45 and an age of 28 days. The form of this *L-d* curve is clearly depicted in Fig. 2.

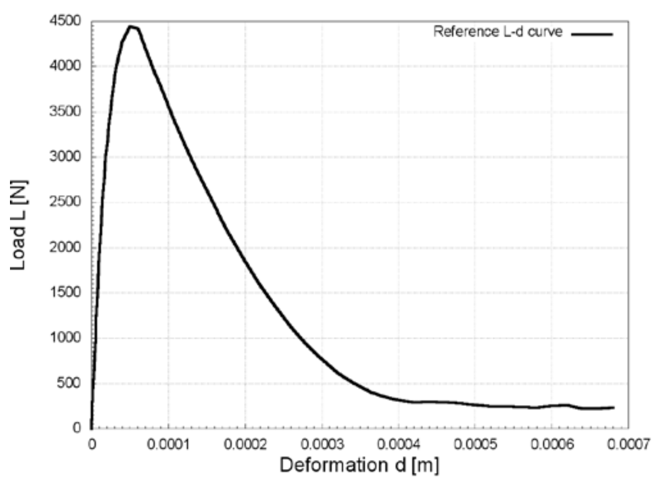

Fig. 2 Reference *L-d* curve from a three-point bending test

III. The Inverse Identification Process

For purpose of the execution of the successful inverse identification of the mechanico-physical parameters of the concrete, a functional computational model had to be constructed on the basis of finite elements, a suitable material model had to be selected and set up, and sensitivity analysis and the global optimization itself had to be carried out, the result of which was the sought material parameters.

A. Nonlinear simulation of a three-point bending test

A numerical simulation of a fracture test was performed in the ANSYS 15.0 computational system in combination with the multiPlas library of nonlinear material models.

Due to task automation requirements, the whole calculation was controlled by a programmed macro which set up the geometry of the computational model and the parameters of the chosen constitutive law, input the solver settings, solved the calculation and finally exported the file containing the points for the *L-d* diagrams. This results file was then used by the optiSLang programme to evaluate similarities with the reference load-displacement curve. Based on this comparison, new sets of design vectors were generated for the sought parameters by a selected optimization algorithm, after which the parameter values of the constitutive law in the macro were replaced by these new values.

B. The computational model

A computational model of a concrete specimen was put together with previously-defined dimensions from a total of 4800 4-node planar elements of the PLANE182 type. The mesh of finite elements was regular and rectangular; the edge length of each element was 3 mm and the thickness was 58 mm. The problem was approached as a plane stress task with predefined thickness. At the location of the notch, two parallel lines were created with a shared node at the top of the notch. With regard to the fact that the monitored area with strongly nonlinear behaviour was located above the top of the notch, and due to the occurrence of local stress peaks in the area above the supports, a linear material model was assigned for the elements at both ends of the computational models within a 30 mm-wide area on both sides of the supports. The final appearance of the computational model is depicted in Fig. 3.

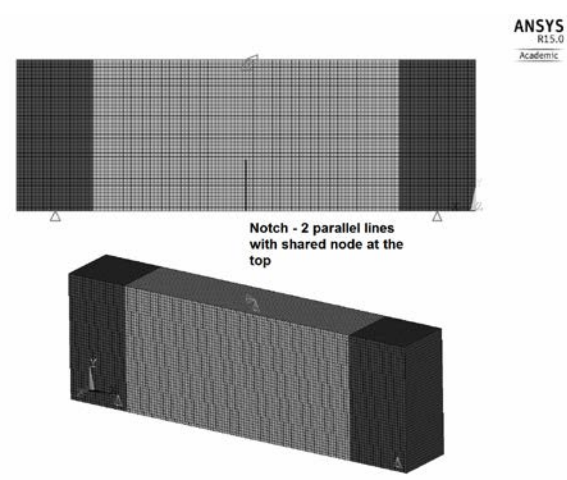

Fig. 3 Computational model

C. The material model

Based on the results of the numerical study [56], which investigated the usability of the selected material model of concrete for the approximation of fracture tests, the material model labelled Menetrey-Willam was selected for the identification of mechanico-physical parameters. The implementation of this constitutive relationship in the used database is based on work published by Menetrey [57], and Menetrey and Warnke [20], and also on a publication by Bazant and Jirasek [58].

This material model belongs to a group of material models of concrete which do not consider the influence of the strain rate on stress, and in which the decomposition of the total plastic strain vector, $\boldsymbol{\varepsilon}_{tot}$, into an elastic component, $\boldsymbol{\varepsilon}_{el}$, and a plastic part, $\boldsymbol{\varepsilon}_{pl}$, is thus expected to take the following form [59]:

$$\boldsymbol{\varepsilon}_{tot} = \boldsymbol{\varepsilon}_{el} + \boldsymbol{\varepsilon}_{pl}. \quad (1)$$

The formula for the yield surface as found in the programme manual [45] has the following form:

$$F_{MW} = A[\sqrt{2}\xi + r(\theta,e)\rho] + \frac{B\rho^2}{\Omega(\boldsymbol{\sigma},\boldsymbol{\kappa})} - \Omega(\boldsymbol{\sigma},\boldsymbol{\kappa}) = 0 \quad (2)$$

with the elliptic function *r(θ,e)* developed by Klisinsky [60] on the basis of Willam and Warnke´s findings [12], which provides the transformation of a circular trajectory with the polar radius ρ into a triple symmetric ellipse [57]:

$$r(\theta,e) = \frac{4C\cos^2\theta + D^2}{2C\cos\theta + D\sqrt{4C\cos^2\theta + 5e^2 - 4e}}. \quad (3)$$

Where $\Omega(\boldsymbol{\sigma},\boldsymbol{\kappa})$ is a hardening/softening function with a work-hardening law and A, B, C, D are model parameters whose form is given by the following relationships:

$$A = \frac{1}{\sqrt{6}}\left[\frac{1}{f_t} - \frac{1}{f_b} + \frac{f_b - f_t}{f_c^2}\right], \quad (4)$$

$$B = \frac{3}{2f_c^2}, \quad (5)$$

$$C = 1 - e^2, \quad (6)$$

$$D = 2e - 1 \quad (7)$$

with

$$e = \frac{f_b\left(f_c^2 - f_t^2\right) + f_t\left(f_b^2 - f_c^2\right)}{2f_b\left(f_c^2 - f_t^2\right) - f_t\left(f_b^2 - f_c^2\right)}. \quad (8)$$

Basic mechanico-physical properties of concrete (uniaxial compressive strength f_c, uniaxial tensile strength f_t and biaxial compressive strength f_b) are present in the given parameters of the model, A, B, C and D in (4) – (8). These strengths have to fulfil the following condition with regard to the functionality of the material model:

$$f_b > f_c > f_t. \quad (9)$$

The inequality between the compressive and tensile strength is satisfied naturally in the case of concrete. The satisfaction of the inequality between biaxial and uniaxial compressive strength can be achieved by rewriting the biaxial strength f_b into the relation:

$$f_b = kf_c, \text{ where } k > 1. \quad (10)$$

The value of parameter k should be around 1.2, according to Sucharda and Brozovsky [61].

Also appearing in (1) for the plasticity surface are coordinates of Haigh-Westergaard cylindrical space, where χ represents the height, ρ the radius and θ the azimuth. The stated cylindrical coordinates can be expressed with the help of the first invariant of the stress tensor I_1 and the deviatoric stress tensors J_2 and J_3 in the following manner:

$$\xi = \frac{I_1}{\sqrt{3}}, \quad (11)$$

$$\rho = \sqrt{2J_2}, \quad (12)$$

$$\cos 3\theta = \frac{3\sqrt{3}J_3}{2\sqrt{J_2^3}}, \quad (13)$$

With regard to the implementation of the angle θ in the formula of the plasticity function, the selected material model differs from models which use the Drucker-Prager plasticity surface. Such models may therefore be unable to approximate the behaviour of concrete correctly in certain loading situations. The Menetrey-Willam material model ranks among those material models with a non-associated plastic flow rule. This statement is supported by the fact that the plastic potential, unlike the yield surface, does not take lode angle θ into consideration [45]. The formula for the plastic potential takes the following form:

$$Q_{MW} = \rho^2 + X\rho + Y\xi \quad (14)$$

where parameters X and Y are again related to uniaxial compressive strength f_c, uniaxial tensile strength f_t, biaxial compressive strength f_b and the so-called dilatancy angle ψ.

$$X = \frac{2f_c\tan\psi - \sqrt{2}f_t}{\sqrt{3}(1 - \sqrt{2}\tan\psi)}, \quad (15)$$

$$Y = \frac{X}{\sqrt{2}} + \frac{2f_t}{\sqrt{3}}, \quad (16)$$

where

$$\arctan\frac{f_t}{\sqrt{2}f_c} < \psi < \arctan\frac{1}{\sqrt{2}} \approx 35.3°. \quad (17)$$

The inequality (17) shown above became a limiting condition in its own optimization procedure.

From the point of view of the use of the FEM, the chosen material model utilizes the smeared crack concept [62]. The given problem was solved with the aid of a softening function based on the dissipation of specific fracture energy G_{ft}, which thus acts as one of the sought parameters. With regard to the need to remove the negative dependence of the solution on the size of the mesh of finite elements, the nonlinear Menétrey-Willam model makes use of Bazant’s Crack Band concept [63]. A complete overview of all material parameters which appear in the used material model are shown in Table 1.

Table 1 Parameters of the selected material model

Par.	*Unit*	*Description*
E	[Pa]	Young's modulus of elasticity
ν	[-]	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
ψ	[°]	Dilatancy angle (friction angle)
ε_{ml}	[-]	Plastic strain corresponding to the maximum load
G_{fc}	[Nm/m^2]	Specific fracture energy in compression
Ω_{ci}	[-]	Relative stress level at the start of nonlinear hardening in compression
Ω_{cr}	[-]	Residual relative stress level in compression
G_{ft}	[Nm/m^2]	Specific fracture energy in tension
Ω_{tr}	[-]	Residual relative stress level in tension

D.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 [64], [65]. As an optimization algorithm was used for the identification of the parameter values of the material model, it was appropriate to use sensitivity analysis as a pre-processing tool with regard to the general effort to decrease the dimensions of the design vector by removing insignificant parameters. Before the implementation of this part of the solution itself, a test set of simulations was carried out by the authors. The results of these calculations were used for the definition of the sensitivity analysis parameters and also for the smooth convergence of the individual nonlinear analyses. The above-mentioned results were represented by a pair of *L-d* curves which delimited the area of interest of the solution from the top and the bottom. The form of the curves is shown in Fig. 4.

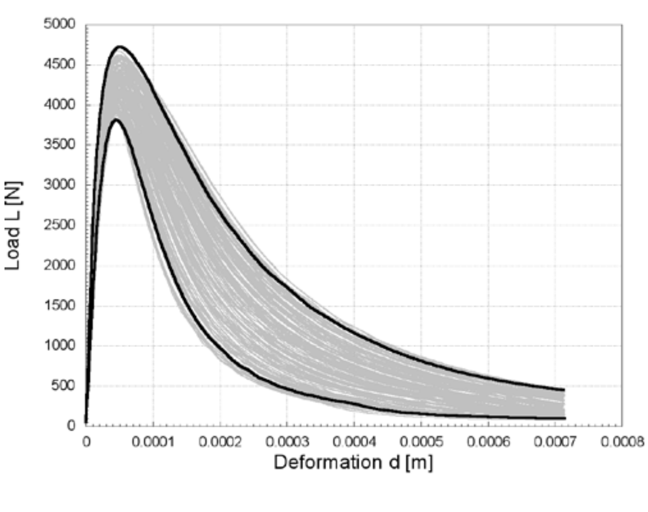

Fig. 4 Delimiting *L-d* curves

The practical use of the data obtained for the purposes stated above consisted in the determination of the extreme limit values of the design variables. The generating of samples in the given pre-tested interval was also the basis for the validity of the assumption of the smooth convergence of the individual solutions.

In order to cover the design space with the needed implementations, the ALHS stochastic method was used [66]. The given method was employed mainly due to the limited number of simulations performed, which was a consequence of the relatively large computation time needed per individual nonlinear solution. The number of realizations was set at 300.

When evaluating the results of the sensitivity analysis it was discovered that it is advantageous for the given problem to interpret the sensitivity analysis results separately for each individual part of the *L-d* curve. Certain input parameters only have a significant influence on the ascending branch, while others only affect the area of softening. As a result, the obtained results were interpreted with regard to the local deviation between the reference and calculated curve at the given part of the interval in question.

The sensitivity analysis proved that the following material model parameters had the greatest influence on the resultatnt form of the *L-d* curve: Young´s modulus of elasticity E, the Poisson coefficient ν, specific tensile fracture energy G_{ft}, and the relative value of residual tensile strength Ω_{tr}. These parameters thus formed the basis for a reduced design vector. Based on the experience of the authors, the following three parameters were also considered as input data within the framework of the subsequent optimization loop: uniaxial tension strength f_t, dilatancy angle ψ and plastic strain corresponding to the maximum load ε_{ml}. The remaining material model parameters were fixed at the mean values of the relevant intervals in the following stages of inverse identification. The original full form of the design factor in the form of:

$$\mathbf{X} = \{E, \nu, f_c, f_t, \psi, \varepsilon_{ml}, k, \Omega_{ci}, \Omega_{cr}, G_{fc}, \Omega_{tr}, G_{ft}\}^T, \quad (18)$$

was thus reduced for the subsequent optimization procedure to:

$$\mathbf{X} = \{E, \nu, f_t, \psi, \varepsilon_{ml}, \Omega_{tr}, G_{ft}\}^T. \quad (19)$$

Apart from the application detailed above, the sensitivity analysis results were also used for the determination of the form of the first generation of design vectors for the subsequent optimization process. Implementations which had the lowest objective function values were chosen for this purpose.

E. Global optimization

After the sensitivity analysis had been performed, the subsequent inverse identification of the material model parameters was carried out using an evolutionary algorithm.

Within the framework of the optiSLang programme, a combination of a genetic algorithm (GA) and an evolution strategy (ES) was used in the given case [67]. This robust method was also selected with regard to the possibility of partial failure when conducting numerical simulations at individual design points. The aim of the executed optimization task was to minimize the difference between the set reference curve and the curve obtained from the FEM simulation of fracture tests. The form of the objective function was thus given by the formula:

$$\text{ERROR} = \sum_{i=1}^{n} (y_i^* - y_i)^2 \tag{20}$$

where y_i* was the value of the force calculated within the framework of the numerical simulation and y_i was the value of the force gained from the experimental *L-d* curve. When tuning the task it was necessary to consider the fact that the fields containing the results of the individual numerical simulations had dissimilar dimensions. This was due to the differing behaviour of the solver when dealing with the individual numerical simulations. This problem was solved using linear interpolation in which the values of the resultant curves were mapped on the basis of the division of the interval in question according to the reference curve. This adaptation enabled the subsequent comparison of corresponding force values.

During the optimization process, inequality design constraints were also used with regard to the need to provide smooth convergence and with the purpose of enabling the Menetrey-Willam material model to function correctly. The form of these conditions was as follows:

$$\varepsilon_{ml} = \frac{f_c}{E}, \tag{21}$$

$$\psi \geq \arctan \frac{f_t}{\sqrt{2} f_c}. \tag{22}$$

The stated design constraints were applied mainly for the reason that the optimization algorithm would purposefully avoid such configurations of the design vector which implied the collapse of the solution within the FEM solver, and which could thus cause early termination of the optimization. Within the framework of the given optimization problem, a total of 30 generations of design vectors were realized with the evolution algorithm. Each generation was composed of 10 design vectors.

IV. Results

The result of the executed optimization was a load-displacement curve whose shape is shown in Fig. 5. The depicted optimum was achieved in 247 iteration. When comparing the shape of this *L-d* curve and the reference curve, it can be said that good agreement was achieved along the whole length of the curve in the described way, and so the relevant material model parameters contained in the reduced design factor can be considered to be the identified mechanico-physical and fracture mechanical parameters of the tested material. The only deviation of a more significant nature to be observed is in the area of maximum loading. The maximum force measured during the experiment was $L_{max,exp}$ = 4441.52 N and the maximum force for the given final numerical simulation reached $L_{max,sim}$ = 4282.60 N, which represents a percentage deviation |Δ| of 3.71 %. With regard to the size of this deviation it can be stated that the level of correctness of the tensile strength value f_t is good.

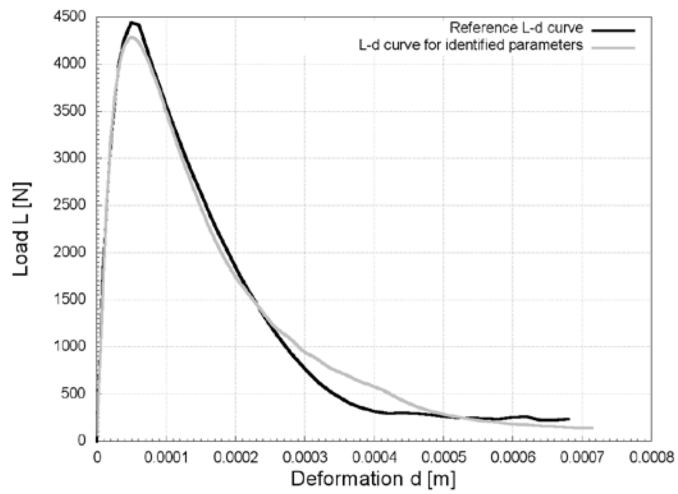

Fig. 5 Comparison of final and reference *L-d* curve

The sizes of the parameter values of the material model are documented further in Table 2. Apart from the final values, the table also shows the values obtained for the pre-optimized parameters which originate from the sensitivity analysis, including the value of the objective function for this set of parameters.

Table 2 Results – final values of parameters

Par.	*Unit*	*Sensitivity*	*Global optimization*
ERROR	[N^2]	1169.3	1029.5
E	[Pa]	$39.3\cdot10^9$	$41.5453\cdot10^9$
ν	[-]	0.213	0.20141
f_c	[Pa]	$48.0\cdot10^6$	$48\cdot10^6$
f_t	[Pa]	$2.388\cdot10^6$	$2.4\cdot10^6$
K	[-]	1.198	1.2
ψ	[°]	10	9
ε_{ml}	[-]	0.001788	0.0021
G_{fc}	[Nm/m^2]	1086	1000
Ω_{ci}	[-]	0.745667	0.75
Ω_{cr}	[-]	0.147667	0.1
G_{ft}	[Nm/m^2]	50	50
Ω_{tr}	[-]	0.0097667	0.00841073

V. Conclusion

The results stated in the previous paragraphs document the usability of optimization methods in the area of the inverse identification of the parameters of nonlinear material models. It has become apparent, though, that when performing the calculations for a specific task such as a simulated three-point bending test, the only parameters that can successfully be defined are those which are utilized in the given loading method. This is thus one of the possible disadvantages of the described method of inverse identification. By lowering the total amount of unknown parameters in the design vector, the computational time was reduced but, with regards to the fixation of insignificant parameters at the mean values of the intervals, these values cannot be considered as having been identified.

In order to completely obtain all the parameters needed for the material model, parameters also need to be identified from experimental data originating from different tests.

An undeniable advantage of the described inverse identification method is the fact that every numerically obtained curve for a certain set of parameters represents a truly converged numerical solution. This demonstrates the functionality and wide range of applications of the selected material model. The following steps can be taken in order to make the presented optimum more precise: (a) increase the number of generations of the design vectors and make the stopping criterion stricter, (b) execute another optimization procedure which uses a different algorithm while using the design vector corresponding to the optimum found earlier as the starting design.

Based on the achieved results, the used material model can be considered to be suitable for the simulation of the nonlinear behaviour of concrete structures. It thus demonstrates that wider options exist for its implementation in the design and evaluation of whole concrete structures.

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