10^{th} International Conference on Fracture Mechanics of Concrete and Concrete Structures
FraMCoS-X
G. Pijaudier-Cabot, P. Grassl and C. La Borderie (Eds)
https://doi.org/10.21012/FC10.234717

A NEURAL NETWORK ENSEMBLE FOR THE IDENTIFICATION OF MECHANICAL FRACTURE PARAMETERS OF FINE-GRAINED BRITTLE MATRIX COMPOSITES

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Key words: Inverse Analysis, Fine-grained Composites, Fracture Parameters, Artificial Neural Networks

Abstract. The paper describes a method for the identification of selected mechanical fracture parameters of fine-grained brittle matrix composites, and its software implementation. The artificial neural network-based inverse analysis method can be employed to obtain parameters from experimental data acquired during three-point bending tests on notched prism specimens. This capability is utilized and extended in order to conduct parameter identification on fine-grained brittle matrix composites. Due to the potentially wide range of composite mixtures and hence the wide range of experimental responses of individual specimens, an ensemble of artificial neural networks was created. It allows the entire range of variants to be covered, and provides resulting parameter values with sufficient precision. Such a system is also easy to expand if a composite with properties outside the current range is tested. The proposed identification system has been tested and employed for the determination of parameters quantifying material resistance against crack initiation and propagation, as well as for the comparison of newly developed composites based on alkali-activated matrix.

1 INTRODUCTION

A great deal of attention has been devoted to the development of inverse methods to determine parameters driving the quasi-brittle fracture behavior of concrete [1]–[3]. The knowledge of mechanical fracture parameters is fundamental not only for nonlinear computational modeling of structures made of quasi-brittle materials, but also for the evaluation of newly developed materials. In many cases, attention is focused on improving the properties associated with resistance to crack formation and propagation, rather than on the maximum strength of the material. One possibility is to obtain mechanical fracture parameters indirectly – based on a combination of fracture tests and inverse analysis [4]. In this paper a methodology of acquiring mechanical fracture parameters of standard concrete using experimental data from three-point bending test and artificial neural network-based (ANN) inverse analysis method is utilized and extended towards parameter identification of fine-grained brittle matrix composites.

The method employed for parameter identification, which combines nonlinear simulations with the training of an artificial neural network, is relatively time-consuming, of high complexity, and requires some knowledge of soft computing methods [4]. Therefore, the whole procedure has been implemented in the

FraMePID-3PB software tool [5] for standard coarse-grained concrete, whose fracture properties are typically evaluated from the response of a notched prismatic specimen with the nominal dimensions $100 \times 100 \times 400$ mm (Figure 1 left), tested in the three-point bending configuration.

The existing identification system has now been expanded to allow the identification of parameters from smaller test specimens with the nominal dimensions $40 \times 40 \times 160$ mm (Figure 1 right), which are typically used for mortars and other fine-grained brittle matrix composites. The aim was to create a robust and extensible identification system that would be applicable to a wide range of materials tested in this configuration. That is why an ensemble of neural networks was implemented into the system, in which the activation of a particular ANN is controlled by the response of the studied material.

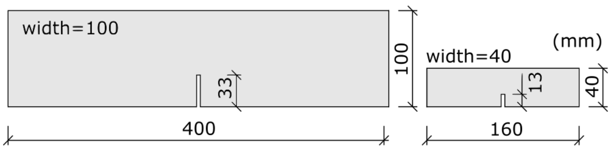

Figure 1: Typical specimen size for coarse-grained composites (left) and fine-grained composites (right) used in a three point bending fracture test.

2 MATERIAL PARAMETER DETERMINATION

2.1 Fracture tests

Mechanical fracture parameter values are determined using the results of fracture tests in suitable configurations (three-point bending, wedge splitting, etc.). In our case, due to the relative simplicity and availability of the testing equipment, three-point bending (3PB) tests were conducted on prism specimens with a central notch. The specimens used for fine-grained composites are typically of the above-mentioned nominal size $40 \times 40 \times 160$ mm. The loading span is 120 mm. In the center of the prism a notch is cut to a depth of about $1/3$ of the specimen depth using a diamond blade saw.

The testing machine has to be stiff enough compared to the tested specimen's stiffness in order to perform a stable test. This is performed with an approximately constant controlled displacement rate, which is chosen so that the maximum load is reached within a few minutes after the start of the test, and which is slow enough to record the post-peak behavior. In the case of the fine-grained composites described in the application section 3, the constant increment of displacement was set to 0.02 mm/min. The deflection of the center of the prism and the corresponding load are recorded until the prism is completely separated into two halves. The outcome of each test is a force–deflection diagram (F–d diagram), which is subsequently used for mechanical fracture parameter determination. An example of a 3PB fracture test configuration is shown in Figure 2.

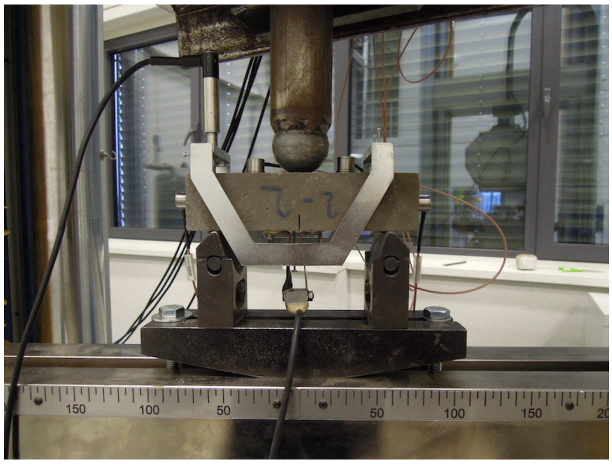

Figure 2: Fracture test configuration.

2.2 ANN-based inverse analysis

An artificial intelligence-based inverse procedure developed by Novák and Lehký [4] transforms fracture test response data into the desired mechanical fracture parameters: $\mathbf{R} \rightarrow \mathbf{P}$. This approach is based on matching laboratory measurements with the results gained by reproducing the same test numerically. The ANN is used here as a surrogate model of an unknown inverse function between input mechanical fracture parameters and corresponding response parameters:

$$\mathbf{P} = f_{\mathrm{ANN}}^{-1}(\mathbf{R}). \tag{1}$$

Conveniently, the ATENA finite element method (FEM) program (Červenka et al. [6]) was employed for the numerical simulation of the fracture test. The 3D Non Linear Cementitious 2 material model was selected to govern the gradual evolution of localized damage. The tensile behavior is governed by the Rankine-type criterion with exponential softening according to Hordijk [7], while the Menétrey–Willam yield surface with hardening and softening phases is used [8] for the behavior in compression. The fracture model employs the orthotropic smeared crack formulation and the rotational crack model with the mesh-adjusted softening modulus both in tension and compression. The analysis is performed under plane stress conditions.

The cornerstone of the inverse method is the ANN which transfers the input data – a response in the form of an F–d diagram obtained from the fracture test – to the desired material parameters. The following three fundamental parameters of concrete are subject to identification: modulus of elasticity $E_{\mathrm{c,ID}}$, tensile strength $f_{\mathrm{t,ID}}$, and specific fracture energy $G_{\mathrm{F,ID}}$. Other parameters of the material model, e.g. compressive strength, were omitted from identification based on sensitivity analysis.

The set for training the ANN is prepared numerically via the utilization of an FEM model (Figure 3) which simulates a three-point bending test with random realizations of material parameters. These are generated with the help of the stratified sampling method and by performing an inverse transformation of the distribution function in order to reflect the probability distribution of the parameter. Rectangular distribution was used for the modulus of elasticity and tensile strength, while descending trapezoidal distribution (Figure 4) was selected for specific fracture energy in order to generate more samples with lower values. This improves the accuracy of inverse analysis for composite mixtures with lower fracture energy values. Its probability density and distribution functions are:

$$f_{\mathbf{X}}(x) = \frac{3b - a - 2x}{2(b-a)^2}, \tag{2}$$

$$F_{\mathbf{X}}(x) = \frac{(3b-a)(x-a) - x^2 + a^2}{2(b-a)^2}, \tag{3}$$

both for $a \leq x \leq b$ where a and b are the lower and upper limits of the fracture energy, respectively, see Figure 4.

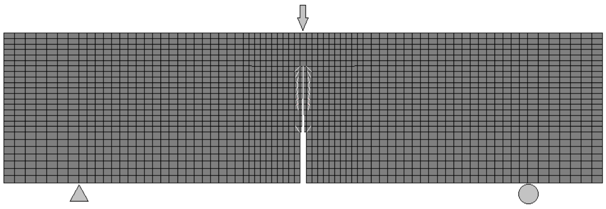

Figure 3: FEM model of the three-point bending test adopted for numerical simulations, including damage distribution at peak load.

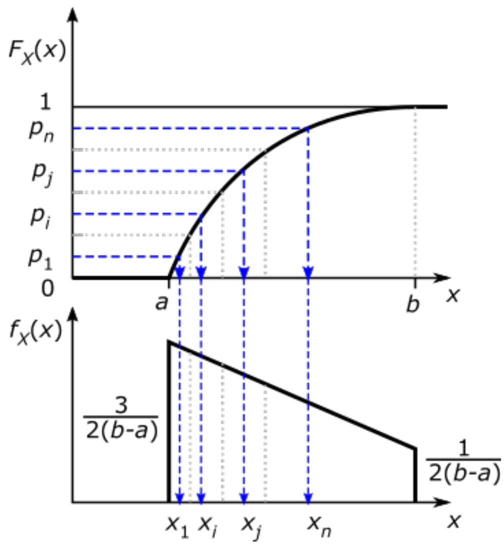

Figure 4: Generating random samples of the specific fracure energy, which has descending trapezoidal probability distribution.

The random responses from the computational model and the corresponding random realizations of parameters serve as input–output elements for the ANN training set. After training, the ANN is ready to solve the main task, which is to provide the best material parameters in order for the numerical simulation to achieve the best agreement with the experiment. This is performed by simulating a network using the previously measured responses as an input. This results in a set of identified material parameters. The last step is result verification – the calculation of the computational model using the identified parameters. Comparison with the experiment will show the extent to which the inverse analysis was successful.

2.3 A neural network ensemble

Due to the potentially wide range of fine-grained brittle matrix composite mixtures and hence the wide range of experimental responses of individual specimens, the decision was made to create an ensemble of artificial neural networks that would cover the entire range of variants and provide resulting parameter values with sufficient precision.

A three-dimensional space defined by three mechanical fracture parameters – modulus of elasticity, tensile strength, and specific fracture energy – is divided into several subspaces, see Figure 5. Every subspace contains a single robust ANN trained for a limited range of parameters. Such a modular system is easy to expand if a composite with properties outside the current range is tested. Figure 6 depicts an example of an identification system with activated ANNs, shown here in a two-dimensional view for clarity.

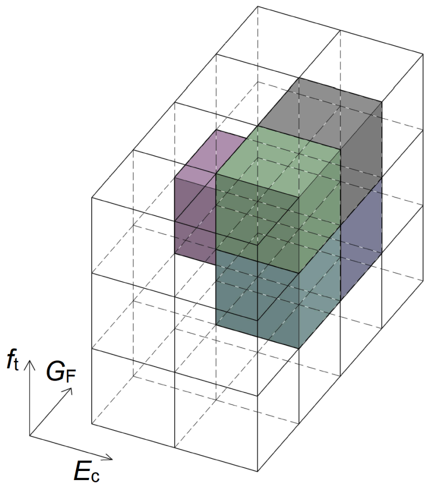

Figure 5: Neural network ensemble-based identification system with examples of active subspaces.

The ANNs in the individual subspaces are of the feed-forward multi-layered type and have the following structure: 3 inputs, 1 hidden layer having 6 or 7 neurons with a nonlinear transfer function (hyperbolic tangent), and 1 output layer having 3 neurons with a linear transfer function, see Figure 7. Each of the output neurons correspond to one of the identified material parameters, and each of the inputs corresponds to one parameter extracted from an F–d diagram. The training set samples were generated using 50 simulations.

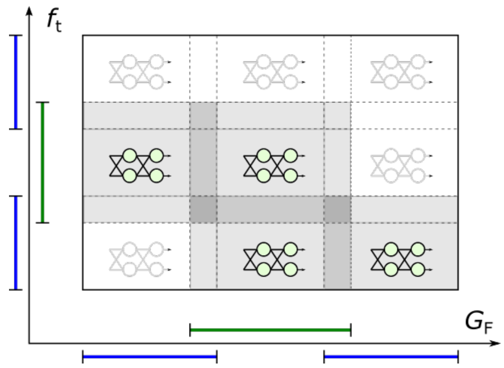

Figure 6: Neural network ensemble-based identification system with examples of activated ANNs displayed in a two-dimensional view.

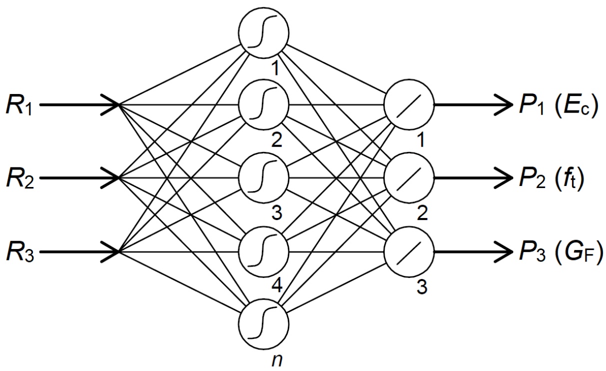

Figure 7: Diagram of the utilized feed-forward multilayer network.

A suitable subspace for the analyzed specimen is automatically selected and the corresponding ANN is activated based on an initial analysis of the experimental response data. The set of mechanical fracture parameters is calculated by simulating the ANN with obtained response parameters.

Sometimes, a specimen has material parameters which are situated close to the boundaries of a subspace and thus may belong to several overlapping subspaces. In this case, the final set of parameters is obtained via the suitable combination of results obtained from all the activated ANNs. It can be calculated as a simple or weighted average. The second method takes into account the fact that the accuracy of an ANN decreases with the distance from the center of its subspace. Figure 8 depicts an example involving two overlapping subspaces: on this occasion it is for the simplified case with a single parameter p.

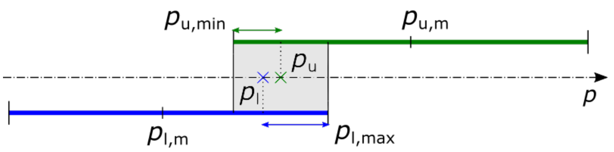

Figure 8: The calculation of weight factors for specimens in the overlapping area of two subspaces.

The final weighted value of parameter p is then calculated as:

$$p = \sum_{i=1}^{n} w_i p_i \tag{4}$$

with $n = 2^k$ overlapping subspaces for k parameters; p_i is the value of parameter obtained from an ANN for the ith subspace (see p_{l} and p_{u} in Figure 8). The weighting coefficient w_i of the ith subspace is dependent on the relative distance λ_i of parameter p_i from its mean point. For the lower subspace l (see Fig. 8):

$$\lambda_i = \frac{p_{\mathrm{l,max}} - p_i}{p_{\mathrm{l,max}} - p_{\mathrm{l,m}}}, \tag{5}$$

For the upper subspace u:

$$\lambda_i = \frac{p_i - p_{\mathrm{u,min}}}{p_{\mathrm{u,m}} - p_{\mathrm{u,min}}}. \tag{6}$$

where $p_{\mathrm{u,min}}$ is the minimum border of the upper subspace, $p_{\mathrm{l,max}}$ is the maximum border of the lower subspace, $p_{\mathrm{u,m}}$, and $p_{\mathrm{l,m}}$ are the means of the upper and lower subspace, respectively. The weighting coefficient is then calculated as:

$$w_i = \frac{\lambda_i}{\sum_{i=1}^{n} \lambda_i}. \tag{7}$$

3 FINE-GRAINED COMPOSITES WITH ALKALI-ACTIVATED MATRIX

Recently, developments in the field have been focused on searching for a material that could be used to replace ordinary Portland cement (OPC) in concrete. This is because of the growing environmental concerns related to OPC production. Extensive research efforts are in progress with the aim of developing new types of binders, environmental-friendly building materials (including alkali-activated materials (AAMs)) which are a promising alternative to traditional cement.

The mechanical properties and application possibilities of AAMs are very similar to those of materials based on OPC. Their major disadvantage is their increased shrinkage during the hardening period, which eventually results in volume contraction, microcracking and the deterioration of tensile and bending properties [9], [10]. The addition of different types of fiber to alkali-activated matrix might lead to a reduced cracking tendency and improved tensile properties for these materials, thus providing them with equivalent characteristics to OPC-based materials [11]–[13].

Currently published works on this topic mainly focus on the determination of the strength characteristics of AMMs, but unfortunately the information on the fracture properties of these composites available in the literature is limited [14]. Therefore, the current research project is aimed at the performance and evaluation of fracture tests on prism specimens made of selected fine-grained composites based on alkali-activated matrix.

The parameters obtained from fracture test records in the form of F–d diagrams can be used to quantify structural resistance against crack initiation and propagation, as well as to compare studied or developed composites based on alkali-activated matrix. They can also be employed for the definition of material models for the deterministic or stochastic simulation of the quasi-brittle/ductile response of composites/members using the Stochastic Finite Element Method model with non-linear fracture mechanics principles. In this case, the recorded diagrams were used as input data for parameter identification and mainly for the verification of the proposed identification system described in the previous section.

For this purpose, two groups containing three sets of specimens were chosen. The first group of specimens were made with alkali-activated fly ash, while the second group of specimens were made with a mix of fly ash and slag as a binder. The first set in each group was a reference set, and these two sets were designated as FA and FAS, respectively. The remaining four sets contained different volume percentages of hemp fibers (0.5 and 1.0 %), designated as FA_0.5, FA_1.0 and FAS_0.5, FAS_1.0, respectively. The hemp fibers were used as a sustainable alternative to the steel and synthetic fibers which are employed to reduce the cracking tendency in alkali-activated fine-grained composites.

In the first group, i.e. power plant fly ash, the sets of specimens were produced from sodium silicate solution (used as an alkali activator), river sand with a maximum grain size of 8 mm, and water and hemp fibers with a length of 10 mm. In the second group, 50 % by weight of the fly ash was substituted by blast granulated furnace slag. Three independent measurements were carried out for each composite mixture. More details about mortar mix design, specimen production and curing conditions can be found in [15].

The variable composition of the mortar mixtures and, in particular, the presence of hemp fibers led to a relatively wide range of responses from the tested specimens, as was confirmed by the recorded F–d diagrams. A total of six ANNs were activated in order to identify the mechanical fracture parameters of eighteen specimens. The set of activated ANNs is depicted in Figure 5.

The mean values (obtained from 3 independent measurements) and coefficient of variation (CoV) of selected mechanical fracture parameters of the FA and FAS specimen sets obtained from the F–d diagrams, i.e. statistics for the modulus of elasticity $E_{\mathrm{c,ID}}$, fracture energy $G_{\mathrm{F,ID}}$ and tensile strength $f_{\mathrm{t,ID}}$ obtained from identification using a neural network ensemble, are summarized in Table 1.

Table 1: Mean values (CoV in %) for selected mechanical fracture parameters of FA and FAS composites.

Parameter	**FA**	**FA_0.5**	**FA_1.0**
$E_{\mathrm{c,ID}}$ (GPa)	19.6	18.5	14.1
	(6.5)	(5.6)	(6.9)
$G_{\mathrm{F,ID}}$ (J/m^2)	54.8	89.0	244.4
	(22.7)	(22.9)	(9.8)
$f_{\mathrm{t,ID}}$ (MPa)	4.7	3.7	2.1
	(4.1)	(15.1)	(12.2)
	FAS	**FAS_0.5**	**FAS_1.0**
$E_{\mathrm{c,ID}}$ (GPa)	23.8	24.1	20.8
	(2.4)	(3.0)	(5.0)
$G_{\mathrm{F,ID}}$ (J/m^2)	50.2	125.8	120.3
	(9.6)	(43.1)	(13.7)
$f_{\mathrm{t,ID}}$ (MPa)	2.6	2.3	2.7
	(7.5)	(12.4)	(8.9)

The identified parameters were verified. The obtained material parameters were used in the computational model and numerical FEM analysis was carried out. The resulting numerical F–d diagrams are compared with the experimental diagrams for both the FA (Figure 9) and the FAS (Figure 10) specimen sets.

4 CONCLUSIONS

For the verification of the proposed identification system, two groups of specimens made from fine-grained alkali-activated composites were chosen. The resulting numerical F–d diagrams obtained by FEM analysis with material inputs based on identified parameters were compared with diagrams acquired from experiments conducted on both FA and FAS specimen sets. Good agreement was achieved between the numerically and experimentally obtained F–d diagrams.

The addition of hemp fibers to alkali-activated matrix should lead to a reduction in the cracking tendency of these materials and improve their tensile properties. For both groups of specimens, the addition of hemp fibers caused a decrease in modulus of elasticity, especially in the case of a higher dosage of fibers. In the case of the FA group of specimens, a significant gradual decrease in tensile strength was observed with the addition of fibers. In the case of FAS, the tensile strength slightly decreased with the addition of 0.5 % of hemp fibers, and for a higher amount of fibers it was similar to that of the reference composite.

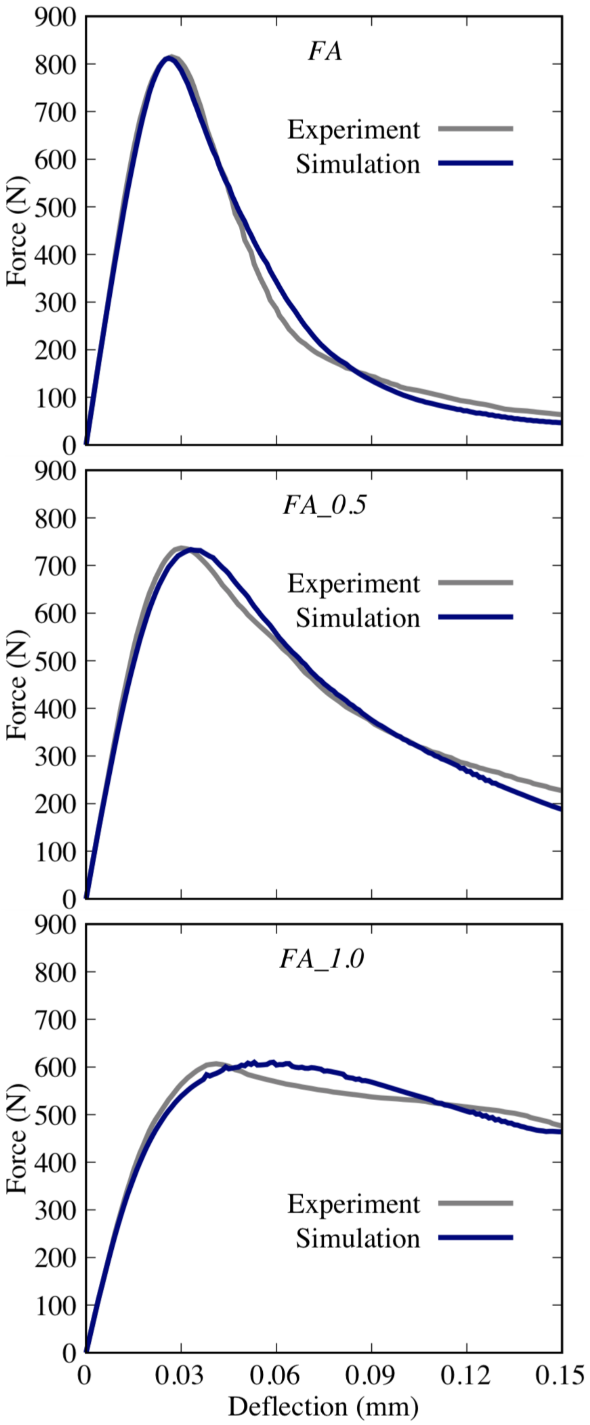

Figure 9: Selected F–d diagrams of FA composite: experiment vs. numerical simulation.

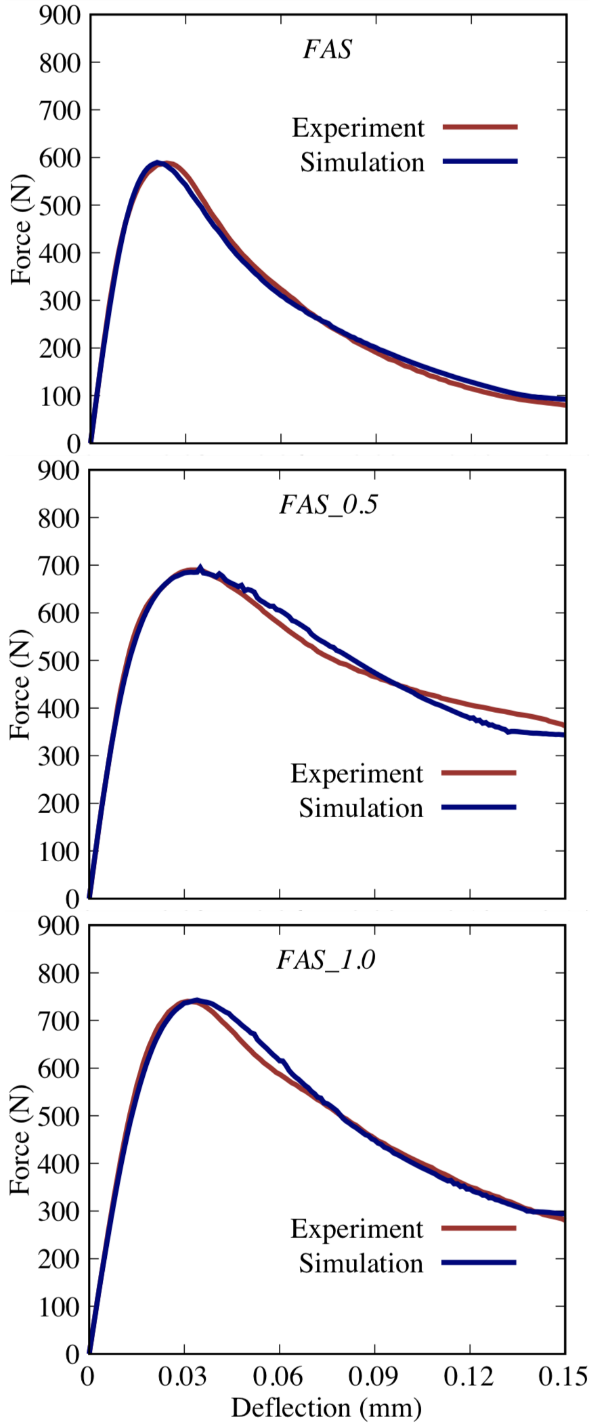

Figure 10: Selected F–d diagrams of FAS composite: experiment vs. numerical simulation.

In contrast, the addition of hemp fibers had a positive effect on the post-peak behavior of both groups of specimens. The fracture energy increased with the addition of hemp fibers to the alkali-activated matrix. In the case of the FA group of specimens, the fracture energy increased more than four times with addition of

1.0 % of hemp fibers. In the case of FAS, the fracture energy increased more than two times regardless of the amount of hemp fibers.

Along with parameter identification using the ANN-based inverse method, it is also convenient to perform the direct evaluation of mechanical fracture parameters from test responses using, e.g. the effective crack length method [16] and the work of fracture method [17]. These provide more complex information regarding the fracture behavior of newly developed composites. Results obtained for the FA group of specimens with these methods can be found in [15]. The trend of the change in the modulus of elasticity and specific fracture energy with the addition of hemp fibers is in good agreement with the values obtained by identification presented in this paper.

The ability of the proposed neural network ensemble-based identification system to identify mechanical fracture parameters of fine-grained brittle matrix composites with variable response while maintaining sufficient accuracy has been confirmed. The collaboration of multiple neural networks for a specimen which occupies a remote region close to the boundaries of multiple subspaces results in more accurate parameters compared to the parameters provided by a single ANN. An important advantage of the system is that it is easy to expand if a composite with properties outside the current range is tested.

ACKNOWLEDGEMENT

The authors would like to express their thanks for the support provided from Czech Science Foundation project MUFRAS No. 19-09491S, project IdeMaS No. FV30244 supported by the Ministry of Industry and Trade of the Czech Republic, and the specific university research project granted by Brno University of Technology, registered under the number FAST-J-19-6040.

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