PREDICTION OF THE MECHANICAL AND ELECTRICAL PROPERTIES OF CEMENTITIOUS COMPOSITES USING ARTIFICIAL NEURAL NETWORKS

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Extended Abstract

Concrete mix design may be defined as a technique of establishing the most cost-effective concrete mixture in terms of the ingredients, while the requirements for the mechanical properties such as workability, strength, and durability are achieved. It is becoming essential in construction due to the rising prices of traditional materials, and recent implementation of alternative materials. In construction of large voluminous structures such as dams, or structures which require high strength of concrete such as high-rise buildings, long bridges, or megastructures, concrete mix design assures that the required properties of concrete are achieved and, at the same time, keeps the use of costly ingredients at the necessary minimum, making the construction as economically feasible as possible. Implementation and application of some novel concrete mix design method is still strictly in the domain of research; however, this work aims to bring it closer to the civil engineering practice. Since the optimal mixtures are usually developed through a relatively long trial-and-error process, making the fabrication a costly venture, this research work focuses on the possibilities of faster and more feasible production. General classification of methods used in concrete mix design includes analytical, semi-experimental, experimental, and statistical methods. This work proposes a method classified as semi-experimental, since it includes both experimental testing and the application of analytical tools, in this case, numerical analysis and a machine learning technique called artificial neural networks. This novel method's goal is to predict the behavior of CNT/CNF reinforced concrete, by incorporating the numerical simulations in ANSYS to substitute laboratory work, and by applying the artificial neural networks to predict compressive strength, flexural strength, and volume electrical resistivity of the cementitious composite material.

Concrete mix design serves to optimize the concrete mixture and explore possibilities of adding materials such as recycled plastic, recycled aggregate, different types of nanomaterials, etc. Most popular nanomaterials used in concrete matrix are carbon black, C60, nano-TiO_2, nano-

Fe_2O_3, carbon nanotubes, carbon nanofibers, and graphene. Nanomaterials are especially attractive as a filler material in the concrete matrix because they may provide additional functions to the concrete, including self-cleaning, self-healing, self-sensing, and others. Therefore, the nano-reinforced concrete composite material presents an excellent choice for multi-functional structures. This work deals with carbon nanotube (CNT) or carbon nanofiber (CNF) reinforced concrete provided with the enhanced mechanical features and the additional ability of internal strain sensing. The ability of self-sensing may be very significant for the development of new sensing systems, and for the structural monitoring field in general. If sensing is possible within the material itself, the monitoring of the structure can be constant and self-sufficient if provided with a powerful processing unit and data storage. Currently, self-sensing concrete is not used in civil engineering practice, partly due to the lack of appropriate sensing equipment and partly due to the high costs of a relatively experimental material. Sensors are devices which respond to physical stimuli by producing an electrical signal where a sensor converts physical parameters into an electrical signal that is further converted to a digital value through a signal conditioning circuitry and the analog-to-digital converter. These components constitute a data acquisition system that processes electrical signals converting them into digital values and enabling further manipulation by a computer. Piezoresistive sensors are based on the piezoresistive effect, using the change in the electrical resistivity of the material when it is deformed under applied strain. Since the CNT/CNF reinforced concrete expresses piezoresistive behavior, it is possible to use it as a piezoresistive sensor.

This dissertation proposes a new mix design method for CNT/CNF reinforced concrete and investigates the possibilities of excluding the experimental testing by applying analytical tools. After the theoretical analysis of the fabrication and behavior of CNT/CNF reinforced concrete in terms of the chemical and electronical aspect, the research focuses on the experimental testing of the composite materials. Thus, the investigation follows the fabrication process regarding the proper nanofiller dispersion, reaching the percolation threshold and electrically conductive networks within the insulating matrix, and finally, providing quality end-product is performed. Experimental work is found in the literature. The observed works use statistical methods to obtain the mixture recipes by varying the weight fraction of the nanofillers which are then tested. Furthermore, the detailed descriptions are provided for the mixture ingredients, nanofiller dispersion, composite fabrication, testing, and the standards which were used for the experiments.

All works have the same type of basic ingredients for the insulating concrete matrix. Namely, Ordinary Portland cement (OPC) containing limited amounts of calcium sulfate (up to 5%) and other minor constituents (up to 5%) with the strength classes of 42.5 and 52.5. OPC represents a basic binding material, and the high purity is chosen so that the possible additional or unexpected factors influencing the properties of the concrete are brought to a minimum. Distilled water is used for the dispersion of nanofillers and tap or distilled water was used for mixing of the concrete. The w/c ratio included the total amount of water used for both nanofiller dispersion and concrete mixing. In accordance with keeping the threatening factors for the concrete quality at a minimum, the used aggregate material is standardized natural or manufactured siliceous sand for the fine aggregate, and gravel or crushed rock for the coarse aggregate. Nanofillers are multi-walled carbon nanotubes (CNTs) and carbon nanofibers (CNFs), both with purity of around 99%. Because of the presence of nanofillers, some additive materials are used to achieve better dispersion and mixing of the materials and avoid phenomena such as segregation, agglomeration, or excessive foaming. Those materials are surfactants, superplasticizers, and/or foam reducing (defoamer) agents. These materials serve to enable a quality dispersion of the nanomaterials, and to allow quality of the concrete mixture. Some dispersions are achieved without the help of any kind of surfactant. Cement pastes, mortars with fine aggregate, or concrete with fine and coarse aggregate are produced within the observed works. Mechanical testing included three- and four- point bending tests, and axial compression test. Electrical testing included two- and four-probe methods. The standards used in the observed works are Eurocode (EN), Indian Standard (IS), American Concrete Institute (ACI), Spanish Association for Standardization (UNE), and American Society for Testing and Materials (ASTM). Out of 49 observed experiments, 13 have been rejected due to the following issues: unclear process of specimen fabrication; unstandardized geometry of the specimens; improper dispersion of the nanofillers (high percolation threshold); pre-dispersed CNTs giving only the weight fraction of the admixture; occurrence of a decrease of mechanical and electrical properties after adding the nanofillers; and determining the tensile strength by a split tensile test. Finally, the data counts 429 mixtures, where 207 were tested for flexural strength, 329 mixtures were tested for compressive strength, and 223 mixtures were tested for electrical conductivity, resistance, or resistivity. These mixtures are later presented to the artificial neural networks as datasets in Group I of the data.

Numerical simulations are employed in this study to establish if it is possible to use ANSYS software as a substitute for the experimental testing of CNT/CNF reinforced concrete specimens. The analyses and simulations are carried out based on the experimental testing. The material models are developed using Material Designer and the results are used to build a comprehensive material library. This material library is later applied in simulations of the mechanical testing of the specimens, namely, three-point bending test and axial compression test in Static Structural. The results are validated by comparison with the results of the experimental testing, taking care of the coinciding geometry and type of the test. Material models are developed using Random UD Composite RVE. The concrete microstructure is heterogeneous and all three aggregate states are present in the concrete mesostructure, however, Material Designer is unable to recognize the various aggregate states of materials. Furthermore, the concrete structure consists of cement and water particles at micro level, while the fine and coarse aggregate materials have the minimum size of 1-2 mm and 2-16 mm, respectively, hence, exist only on the macro scale. This occurrence cannot be described within Material Designer. Due to the limits of the Material Designer, the concrete matrix is not modeled as composite of all ingredients, but as a homogeneous material. The Random UD Composite RVE is defined by the geometry of the fiber, including the fiber volume fraction, mean misalignment angle, seed, fiber diameter, and the repeat count. Parametrization is done for the fiber volume fraction, so that each composite group is prescribed with the suitable values. The duration of RVE generation and meshing depends on the seed and the repeat count parameter. It is established that for the smaller fiber weight fractions, from 0.01-0.1 wt.%, it is better to use smaller mean misalignment angle and repeat count, while the seed should be kept between 15000 and 25000. For the weight fractions higher than 0.1 wt.%, the mean misalignment angle can be increased to 5, or even 10 for fractions over 1 wt.%. The seed should increase steadily in line with the fraction, going up to around 70000 for 2 wt.%. Only conformal meshing is used, without a limit for the maximum FE size. It is established that limiting the mesh size leads to difficulties for the model to provide a complete mesh between the matrix and the fiber materials. Conformal meshing coincides with the relatively irregular geometry between the two materials.

After homogenization in Material Designer, the density and tensor of elasticity of the isotropic material is provided for the Engineering Data. Space Claim is used to build the geometry of specimens for the compression and bending tests, following the realistic testing set-up for the axial compression test and for the three-point bending test according to Eurocode. Hence, bending test specimens are small beams and the compression test specimens represent the halved small beams. The Mechanical part of the Static Structural model defines the meshing of the model, supports, loading, and analysis' settings. Meshing of both types of specimens includes hexagonal finite elements (Hex8, Hex20) of 2 mm, type SOLID185. Linear SOLID185 elements are 8-node three-dimensional finite elements used for thick shell and solid structures. Analysis of the meshing element number and quality shows that all elements in both compression and bending model have the same size and shape. The FE size is 2 mm in both cases; therefore, the compression model has 8000 elements, and the bending model has 16768 elements which ensures relatively quick static analysis. Simulation of the loading is indicated by the ultimate strength of the referential plain concrete material from the experimental testing. Compression test set-up implies that the entire bottom surface is fully supported and that the entire top plane is loaded. The loading of the model is presented as the displacement of the top surface, which is input as tabular to ensure the steady growth of the stresses. The analysis of the stresses is provided with sub steps within one second of the implicit static analysis. The minimum number of steps is 10 and the maximum is 20, to ensure incremental analysis but keep the speed of convergence. Bending test model includes additional bodies in the form of supports and the impactor. The contact surfaces between the support bodies and the beam are defined as "no separation" contacts, where the bodies are fully connected with allowed sliding. Displacement is set to zero in all global directions for both supports. Even though statically, the constraints are in vertical and horizontal longitudinal directions only, this setup helps the software to converge quicker and easier. The impactor body transfers the force from the moving loading press to the beam. Therefore, the contact type between the impactor and the beam is "bonded" and the vertical displacement is provided at the top surface.

Results of the static analysis are represented with the maximum, minimum, and the average values of the maximum principal stress, the minimum principal stress, and the normal stress. It is observed that in some cases Young's modulus of the composite material is even higher than 200 GPa, and the bending strength surpasses the value of 20 MPa. It is safe to say that this is an overestimation, and that it would not occur in realistic conditions. However, the results show somewhat realistic material behavior for the composite materials with the weight fractions of up to 0.1%. Thus, for the lower weight fraction of the nanofiller, the results seem promising and imply further research. As for the weight fractions over 0.1%, it may be concluded that the microstructure should be modeled thoroughly from the bottom up, considering individual constituent materials and modeling the nanofillers more realistically in terms of their interaction with each other and within the concrete matrix. Similarly, the compression test results scarcely show a realistic situation. Although there is an increase in strength in most cases, this increase is not the realistic value which the nanofillers actually provide to the concrete matrix. It may be observed that the compressive strength is changed negligibly, with the increase maximum of 1 MPa. Experimental research included less variations of the nanofiller weight fractions, hence, the validation is implemented for the total of 51 cementitious mixtures, including plain and nano-reinforced concrete. All observed experimental investigations included the specimens with the same geometry (40×40×160 mm) and the type of testing (3-point bending). It may be observed that the difference between the experimental testing and the numerical simulations of the plain concrete mixtures, as well as the nano-reinforced mixtures is much higher than for the compressive strength, going as high as around 110%. This occurrence cannot be considered possible. There is no evidence so far that may show such high increase of strength, regardless of the additional materials or the method of fabrication of the composite material. Hence, the flexural strength results from the simulations are not realistic and therefore should not be considered acceptable. Nevertheless, the results from the numerical simulations are used for further analysis by the artificial neural networks. Total of 164 mixtures are presented to the ANNs as datasets of Group II.

Machine learning methods can establish the nonlinear dependencies between the effect factors through minimizing the error via the regression with a remarkably high accuracy of results. Although there are many machine learning techniques and even more types of each technique, as well as the combinations between them, this work focuses on the basic programming of artificial neural network models to provide the basis into further investigation of the application of machine learning in the optimization of mix proportions of CNT/CNF reinforced concrete. Artificial neural networks are developed in Matlab R2020b, using neural fitting tool and the script editor. The networks are trained using both experimental results (Group I) and numerical results (Group II) to establish the applicability of these methods in the civil engineering practice. The models are built using the NF tool and using the script directly. After testing the ANN models from each group, the results and behavior of the ANN models are compared to establish the viability of using the results of ANSYS simulations instead of the experimental testing results. Architecture of ANNs includes the number of layers and the number of neurons in each layer, as well as the algorithm type and the activation function. In this work, all neural network models have constant learning parameters in order to provide a proper comparison of models within both groups. By fixing the learning parameters while varying only the number of the hidden neurons and the subsets ratios, it should be possible to establish which type of architecture presents the best fit for each group and subgroup of models. Total number of layers in all ANN models is three, including the input, one hidden, and the output layer. This type of architecture is called the "shallow" network, and it is commonly used for relatively small datasets regarding the number of input neurons and data tuples. Number of hidden neurons is connected to the number of neurons in the input layers. This work uses two dependencies given in the literature and proposes an additional dependency to test and observe the behavior of the models. Neural network models are developed additionally by direct manual scripting in Matlab R2020b. This way, more options are available in terms of architecture and the process of training and optimization. All ANN models are initially trained using 80% of the full dataset, which is applied only for training and validation. The validation is used at this point to halt the training process, and the training/validation subsets are set to the ratio of 85/15 for the initial and optimization stage. During the initial stage, the number of hidden neurons is equal to the number of input neurons. Later on, it is adjusted based on the results of the optimization and testing. After the initial training, the topology is optimized by iterating the number of neurons in the hidden layer from one to $3 \cdot Ni$, respectively. Optimization of the initial model establishes the optimal number of neurons in the hidden layer. Improved topology of the network implies better generalization and contributes to the stability of the network. The optimization is indicated via the level and the change of the mean squared error for varying number of neurons in the hidden layer. Then, two values are chosen to be tested further based on the optimization results. These two models are tested with the rest 20% of the dataset and based on the results of the testing, a single topology is chosen as the final working model. The final working ANN model is then trained using the complete dataset and without any restrictions. It means that the training continues until the minimum training gradient of 10e-7 is reached. If the gradient is not reached as the training reaches a thousand iterations, it is immediately halted.

Results for the total regression coefficient lower than R=0.8 are considered unsatisfactory. Evaluation of ANNs is provided for the models developed using NF tool which have shown the best behavior. Datasets are randomly divided into two subsets according to the ratio of 80/20, using the 80% of the respective set for repeated training and subsequent testing using the rest 20% of the set. Sensitivity analysis shows absolute or relative contribution of each input parameter to the output value. It may also influence the topology of the final working model because it may show that some parameter could impair or slow down the learning process. On the other hand, it shows which parameters are crucial. This work uses the weights method, otherwise known as the Garson's algorithm. The algorithm is specifically created for supervised neural networks with a single output to describe the relative importance of the input parameters by deconstructing the model weights.

Models from the datasets which give the mechanical properties as the output, show satisfactory results with the regression coefficient values higher than 0.8. For the prescribed models for both Group I and Group II, the most regular error distribution is obtained when the number of hidden neurons equals the number of input neurons. Other occurrence shows that the model which has number of hidden neurons equal to $Nh=2Ni+1$, exhibits the best behavior within its subgroup. Nevertheless, models with $Nh=3Ni$ also showed comparable behavior to other models, confirming the hypothesis of this work. Since these models show satisfactory results, the evaluation was performed. R values of the evaluation models are compared to the results of the initial training. In some cases, regression coefficients of the evaluation models are higher than the initial R values. This may occur due to the favorable distribution of tuples during randomization or the fact that the evaluated models are trained on a smaller dataset. That said, the difference between the values does not exceed 0.1, meaning that the validity of the initial models is confirmed. Evaluation of the initial models concludes that all models showed satisfactory behavior with the given topologies.

Response of the ANN models which were developed using the script editor in Matlab R2020b, are observed at each stage of the development: initial, optimization, testing, and working stage, respectively. Each dataset is used for one model development throughout the former stages. the initial topology included equal numbers of input and hidden neurons. Results are satisfactory for all models with the mechanical properties as output. Nevertheless, the topologies are optimized. The optimization consisted of iterative change of the number of neurons in the hidden layer, beginning from one and ending at the value of three times the number of input neurons, and following the change of the root mean squared error for training and validation. Testing of the optimized models is provided for the topology which has given better response of the network during the optimization process. The testing is performed with the simulation function using the

20% of the full dataset. After testing, final working models are trained using the full respective dataset. Training is performed without any other subsets, as it has been previously described. It may be observed that regression coefficients for all models are very high, with R>0.99, when the learning process is not limited with anything else other than the learning gradient and number of iterations.

The prescribed models from the dataset with electrical resistivity as the output (RESIST) gave the regression coefficient values much lower than the expected 0.8 limit, which is deemed unsatisfactory in this work. Further investigation is made to try to establish the source of this behavior. Therefore, the RESIST dataset was revised. The previous experimental results which were showing that the percolation threshold is not reached have been omitted from the dataset with the assumption that the training of the networks was unsuccessful because of the incoherent behavior of samples. Also, the results which showed relatively higher resistivity for higher weight fraction of the nanofiller compared to other samples within the same sample group were rejected as outliers. Furthermore, the input neuron which gave the cross-sectional area of the sample was added, in order to try to enrich the network with more learning points. After the revision was complete, the new dataset was normalized in the same manner and prepared for training. Other than the increase of the number of input neurons and thus the number of hidden neurons, there was no other changes to the twelve new models. Results of the revised RESIST models show that the behavior of the models has not improved after the revision of the initial dataset. Possible explanation could be that the referential samples without nanofillers may be considered as outliers for the overall dataset. For example, within one sample group, value of the resistivity of the plain sample is 7700000 Ωcm, while the resistivity after reaching percolation threshold with 0.048wt% of CNTs is 360000 Ωcm. Hence, the referential non-reinforced sample may be considered an outlier of the dataset. This assumption would imply that the dataset needs further revision, however, further revision would compress the dataset to the point of instability of learning because the total number of tuples would be around 100. Thus, it would be best to make a comprehensive experimental investigation to obtain more stable results. The scripted models for RESIST dataset showed similar behavior, where the R values are slightly higher but still under the value of 0.8, and thus unsatisfactory.

This investigation included the multi-physics approach in addressing the application of numerical simulations and of artificial neural networks for predicting mechanical and electrical properties of CNT/CNF reinforced cementitious composite materials. The following conclusions may be defined. *Mechanical and electrical properties are improved by the presence of the CNT or CNF nanofiller.* It has been shown that if proper dispersion is achieved, and the mixing and molding of the concrete is made according to the standard, the mechanical properties of the composite material are significantly improved. *Numerical models of CNT/CNF reinforced concrete cannot realistically respond to mechanical stimuli.* ANSYS models of the CNT/CNF concrete composite material showed promising results only for up to 0.1 wt.% of the nanofiller. *Mechanical behavior of CNT/CNF reinforced concrete may be predicted using artificial neural networks. Electrical behavior of the CNT/CNF reinforced concrete cannot be predicted using artificial neural networks.* The lack of comprehensive information on the electrical behavior of these materials, leads to insufficient learning materials for the neural network. It is shown how only false positive results may be achieved. Finally, *number of neurons in the hidden layer of the ANN equal to* $N_h=3 \cdot N_i$ *may provide valid predictions.* The assumed value of the number of hidden neurons shows very good results and does not exhibit overfitting of the networks in this work.

The idea of this work is that the application of numerical simulations and artificial neural networks for material design and prediction of the behavior of CNT/CNF reinforced concrete could be the basis of a new mix design technique which will minimize or completely exclude the use of time-consuming and costly experimental testing. To this goal, the abovementioned issues regarding the electrical behavior and material modeling of the composite materials should be resolved. Proposal of further work implies performing a comprehensive experimental testing of the electrical properties keeping constant the laboratory and experimental factors. Moreover, establishing a suitable software which can support the microstructural modeling and encompass the concrete's mesostructured, would resolve the issue occurring within ANSYS and provide simulations of the electrical testing as well.

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