Review Report on the PhD thesis submitted
to the Faculty of Civil Engineering and Transportation of Silesian University of Technology

to attain
the title of Ph.D. – Doctor of Philosophy in Civil Engineering
(tytuł doktora nauk technicznych w dysyplinie inżynieria lądowa i transport)

entitled
"Prediction of the mechanical and electrical properties of cementitious composites using artificial neural networks"

Author: **MSc. CEng Sofija Kekez**

Supervisor: **Prof. Jan Kubica, PhD, DSc. CEng.**
Assistant supervisor: **Dr. Marcin Górski, PhD, CEng.**

The doctoral thesis was prepared by MSc. CEng Sofija Kekez, and submitted to the Faculty of Civil Engineering and Transportation of the Silesian University of Technology to attain the title of Ph.D. – Doctor of Philosophy in Civil Engineering.

The legal basis for the review is The Act of July 20, 2018, Higher Education Law and Science (with later amendments).

The presented review report is organised into seven sections:
I) Profile of the Candidate
II) General description of the manuscript
III) Project background and its purpose
IV) Evaluation of the literature used
V) Detailed substantive evaluation of individual parts of the dissertation
VI) List of queries
VII) Final conclusion and evaluation statement

Profile of the Candidate

The Candidate **MSc. CEng Sofija Kekez** has completed her Master's degree in the Department of Civil Engineering and Geodesy, Faculty of Technical Sciences, University of Novi Sad, Serbia (2017). According to the information provided, the Candidate has not previously applied for a doctoral degree in Poland or abroad.
After her Master's degree, in 2018, Sofija Kekez was awarded of PhD scholarship supported by "SymIn" – Simulation in Engineering, Interdisciplinary PhD studies, the Silesian University of Technology [project number POWR.03.05.00-IP.08-00- PZ1/17].
She is an Autor of eight and co-author of five publications (in three as the first Author). She has presented her works during nine conferences, among others: Numerical Modelling Strategies for Sustainable Concrete Structures (SSCS 2022), Marseille, France; 6th International Conference on Structural Engineering and Concrete Technology (ICSECT 2021), June 2021, Lisbon, Portugal 66. Konferencja Naukowa Komitetu Inżynierii Lądowej i Wodnej PAN oraz Komitetu Nauki PZITB, September 2020, Krynica.

General description of the manuscript
This PhD thesis manuscript is written in English and consists of 9 main chapters. It comprises 149 pages, a list of symbols and abbreviations, a bibliography list of tables and vast appendices of 138 pages. It begins with an introduction to the subject, which presents the background and motivation of the research.
Chapter II consists of a literature review and Chapter III includes a theoretical background based on 154 publications. The literature review is followed by Chapter IV, presenting assumptions and hypotheses. Chapter V the experiments and testing procedures reported in the literature were presented. Chapter VI and Chapter VII introduce the reader to numerical analysis and simulations, and artificial network models that were employed by the Candidate. That part is followed by Chapter VIII, summarising the results, and chapter 9 shows future research directions based on the Candidate's studies.

The manuscript is prepared in appropriate editing standards. All the figures are carefully designed and presented in the text. The manuscript's language is coherent, the ideas are presented clearly, and the document reads easily.

Evaluation of the literature used.
The literature used as part of the doctoral dissertation is correctly selected. Moreover, it is varied and rich. It is worth emphasising the ability to use the latest literature on the subject and numerous references to the newest world research on the subject matter. The Candidate used 154 scientific bibliographic items. The latest publications issued in the last 5-6 years (since 2016) constitute 44% (68 items) of the total literature, which in the high current dynamics of knowledge circulation in science is a satisfactory indicator.

Project background and its purpose
In the doctoral dissertation, **Ms Sofija Kekez** refers to the issue of the application of nanomaterials: carbon nanotubes CNT and carbon nanofibers CNF in concrete. The main advantages of such addition are enhanced mechanical properties and higher electrical conductivity. The concrete with such features gains new potential applications and becomes multi-functional with self-sensing ability. The ability of self-sensing may be significant for developing sensing systems and structural monitoring.

As the optimal mixture of CNT or CNF reinforced concrete is usually developed through a relatively long trial-and-error process. Remembering that CNT and CNF are costly ingredients, the Candidate is exploring the application of numerical simulations using artificial neural networks (ANN) for the material design process and properties prediction. The main goal of the work is to minimise the use of time- and cost- consuming experimental testing. By implementing the novel concrete mix design approach and verifying its potential for the designing of self-sensing concrete, Autor is hoping that self-sensing concrete will become more feasible and cost-effective. This design procedure may increase the application of this type of concrete in civil engineering.

This dissertation presents novel methods of predicting the behaviour of CNT and CNF reinforced concrete, including numerical simulations of the composite material in ANSYS and the application of artificial neural networks for predictions of compressive strength, flexural strength, and material electrical resistivity.

Detailed substantive evaluation of individual parts of the dissertation

Chapter I of the thesis introduces the reader to the research context, motivation, methodology and outlines. In this part of the manuscript, the Candidate clearly presents five dissertation objectives:

1/ Forming a comprehensive collection of carbon nanotubes and carbon fibre reinforced concrete experiments, including all possible factors affecting the final performance of the composite material.
2/ Developing numerical models and simulating performed experiments to establish a possible alternative to traditional concrete mix design methods.
3/ Establishing if numerical models are capable of emulating the concrete fabrication process and testing.
4/ Developing artificial neural networks for predictions of the compressive strength, the flexural strength, and the electrical volume resistivity of the self-sensing cementitious composite materials.
5/ Establishing the optimal type and architecture of an artificial neural network for this type of problem by varying the parameters of the network.

I judge the purpose of the work as quite ambitious; it includes the selection of the experimental works that deal with the fabrication and testing of self-sensing cementitious composite materials, selection of the factors that affect the properties of the material. Moreover, it included developing a model in ANSYS and design, test and calibration of the architecture of artificial neural networks.

Methodology selection was appropriately presented and discussed. The Candidate explains in Chapter I, that work was divided into two main parts. The first part of the work consisted of collecting the data related to carbon nanotubes, and carbon nanofibers concrete fabrication processes, including the processes of the nanofiller dispersion in the matrix, mixing, moulding, and curing.

The second part considers the application of numerical simulations of the material design and the testing of the specimens bending and compression as an alternative to the experimental procedures using ANSYS software. The materials are designed, and experiments are reproduced to observe the possibility of using this software. The obtained results of the simulations results are collected and used to develop artificial neural networks designed to predict concrete material behaviour.

Chapter II gives the literature review related to the concrete mix design and the artificial neural networks. The description of design methods brings the methods of analytical, semi-experimental, experimental, and statistical methods closer. Reading this text leaves a significant insufficiency resulting from the lack of the presentation of the primary analytical design method, the method of three equations, with an explanation of its principles.

Moreover, it should be noted that the Candidate does not mention the methods of designing a concrete mix, which she probably encountered and familiarised herself with while working in a Polish research team. In Poland, the most frequently used methods of designing concrete composition include mentioned method of three equations, the method of successive approximations (Kuczyński's method), and the method of two-stage gravel cover (Paszkowski's method).

In Chapter II, the Candidate enumerates and describes more advanced techniques that are dedicated to designing self-compacting concrete based on rheology and cites the works of the research group that uses genetic algorithms and extreme learning models (ELM). In this development, the exclusion of the need for laboratory work is predicted, with no need for trial batching. In my opinion, this is an overly optimistic statement and very far-fetched. Today, it is not easy to imagine the fabrication of concrete structural element with concrete designed in such a way, made directly in the concrete mixing plant and sent on-site without any trial batch production ...

Chapter III is in fact, the continuation of the state-of-the-art. Among others, subchapter 2.1 seems to be a continuation of the STAR presented in Chapter II where standards and methods in concrete mix design are presented. Similarly, we find this section's continuation of the STAR on artificial neural networks. The presentation of the state of art on this topic in two places is confusing for the reader.
In my opinion, a summary of the information on the Fundamentals of electronic (*electric?*) (Ch. II, 1) should be introduced after the subchapter on self-sensing concrete.

In subchapter 3 Self-sensing concrete, the Author has enumerated functional fillers that have been proved effective for providing the sensing ability: carbon or steel fibres, carbon nanotube, carbon nanofiber, carbon black, nano-SiO_2, nano-TiO_2, nano-Fe_2O_3, nickel powder, graphene, or a combination (hybrid) of several. For what reasons has Autor limited herself in this study to carbon nanotubes and carbon nanofibers?

You have mentioned that "mechanical and other properties of carbon nanotubes are greatly superior in comparison to any traditional civil engineering material" the comparison between concrete tensile strength and carbon nanotubes is provided, showing the potential of carbon nanotubes 11000-100 000 [MPa] to improve concrete tensile strength 2-5 [MPa]. We expect those revelations to be followed by information about the reinforcing capacity of nanotubes and nanofibers on concrete and examples showing the effect of the addition of CNF/CMT on concrete properties. The comparison of properties of nanotubes and concrete - thermal conductivity 2000-6000 [W/m·K] vs 1.0-1.8 [W/m·K]; electrical conductivity [S/m] 10^2-10^6 compared with 10^{-8} the expected improvement of self-sensing capacities of such composites is well understood.

Nevertheless, one of the main shortcomings of the thesis is the lack, in this section, of data presenting the influence of nano-addition on concrete properties**.** In the document, we find no comprehensive description presenting the relation between the amount of nanofiller and the basic properties of concrete mechanical and electrical.

Section 3.3 of Chapter III introduces the concept of the percolation threshold and the critical concentration of the filler to reach this threshold. It is written that "(…) The effective concentration is not higher than 1.5% for the fibrous filler, whereas it is at least 5% for the particle filler(…)" – please state if this refers to mass or volume? Unfortunately, there are no references to most statements presented in this section.

Section 3.4 highlights the issue of nanofillers dispersion, an important aspect that may compromise the homogeneity of the concrete and lead to segregation and strongly affect concrete sensing properties. The influence of the concrete mix components on w/c ratio, coarse aggregates, and mineral additives was discussed in this section. Section 3.5 Properties of self-sensing concrete and 3.6 .

Mechanisms of electrical conduction in self-sensing concrete this ten-page section (from 3.4 to 3.6) is based mainly on book reference 67 ([67] Han, B., Xu X., Ou, J. Self-Sensing Concrete in Smart Structures, 2014, Butterworth-Heineman). Are there any missing references to original sources of information in the text?

Subchapters: 3.6. Mechanisms of electrical conduction in self-sensing concrete and 3.7. Measuring the sensing property of self-sensing concrete should also be moved to the section where electric properties are discussed.

Subchapter 4 introduces numerical simulations that the Candidate will undertake using FEM (ANSYS) to analyse the mechanical behaviour of carbon nanotubes CNT and carbon nanofibers CNF concretes (in fact, small aggregates concretes – mortars). The information presented in this section in fact, belongs to Chapter VI, Numerical analysis and simulation.

Subchapter 5 describes the artificial neural network method, types, levels of layers, networks, way of extrapolating outputs, and dataset normalisation.

Chapter IV presents the assumptions regarding experimental research data in 35 papers selected for evaluation by the Candidate and also the hypothesis made about numerical simulations. I am very positive about the Candidate's critical assessment of the assumptions made and of the input data and limitations of tools used for modelling. Nevertheless, most of the hypotheses presented on page 60 are self-evident and sounds obvious. In your opinion, which of them were the least obvious and the most difficult to prove?

The title of **Chapter V** Experimental research is misleading. One would expect the results of the Candidate's experimental work to be presented in this section. Chapter V reports in fact the experimental research work programs of each treated reference source. It includes dispersion of nanofiller, and fabrication procedures: including mixing, moulding and curing. Moreover, information about the way of evaluating the quality of the nanofiller dispersion in the matrix has been analysed. Apart from the general composition of selected mixes, there is no information about the quantitative proportion of components. Moreover, in table 5.3, no information about the quantity of CNT and CNF was provided. Was that information not required as input data for the model?

In **Chapter VI** Numerical analysis and simulations were performed using the ANSYS software package for CNF and CNT concrete compositions from the literature.

Page 79, Subchapter 4 Results - "(…) It may be observed that the cracking did not occur in any of the composite material specimens. That is also confirmed by the fact that Young's modulus and Poisson's ratio of all homogenised composite materials increased significantly with the addition of the nanofiller (...)". This statement compromises the results of numerical investigations and may be evidence of incorrectly adopted assumptions. The modulus of elasticity of cementitious

material higher than 50 GPa is challenging to be accepted even as the numerical result. Similarly, the tensile strength of 10 MPa when compressive equals 30 MPa. These results shall be further processed with the necessary review of the input data.
Page 83 - "(…) Similarly, to the results of the bending test, the compression test results scarcely show a realistic situation" (…) If so, should they be presented in the doctoral thesis?

Page 83 - What Autor means by stating (…) The figures are divided between similar mixtures of cement, mortar, and concrete (…)"

It's worth noting that by summarising the results of numerical simulations, the Author critically addresses their values.

Chapter VII presents the developed and optimised neural networks model. The experimental results and the numerical simulations were undertaken, and sensitivity analysis was done to establish the optimal artificial neural network development procedure and its architecture. From the way this section is presented, we can deduce that it is the Author's specialisation. She is at ease in this subject, presenting the following stages of the process: artificial neural network training, validation, and testing process.

The numerical work and ANN modelling work is summarised in **Chapter VII.** It was concluded that ANSYS Material Designer is a useful tool for the investigation of CNT or CNF concretes properties and strength with lower weight fractions of the nanofiller material (weight fraction to 0.1%). For the amounts above 0.1% model gave unrealistic results in terms of the flexural strength and Young's modulus. Moreover, the compressive strength showed a variation of these values (increase or even decrease) for higher weight fractions, which does not coincide with the reported results.

List of queries

1) You have presented several concrete design methods in your PhD thesis. Which of them were finally selected, and how the designing methods were implemented in your model? Could you refer to the method of three equations and provide your opinion about its application to designing carbon nanotubes and carbon nanofibers modified concrete?

2) Carbon and steel fibres are less expensive and provide conductivity improvements in concrete. Please explain your choice and reasons why you have limited your work to CNT and CNF.

3) How do you estimate the actual capacity of CNF and CNT to reinforce concrete? In your opinion, what is the satisfactory level of cement composite reinforcement that would justify the use of the modification with the addition of CNF and CNT?

4) Page 133, Figure 7.5.30 presents the Contribution of the input parameters to the output value. Please explain the coded input parameters shown on the pie charts during the presentation. How was the input parameter's relative influence (weight) on the output determined? Arbitrary?

5) Machine learning efficiency depends on reliable input data. In the papers that you have considered the mechanical properties, the three-point bending and compression tests were tested on variable geometry specimens (page 70). In your opinion, how does the data obtained on different sizes of specimens influence the results? What is the specimen size effect of concrete strength, and how may this influence your simulations?

6) Do you see any possibility of achieving greater consistency between the model and experimental results? What could be the potential sources of error generating such anomalies (Young modulus of concrete 200 GPa, the tensile strength of 10 MPa when compressive equals 30 MPa)? How to avoid such discrepancies with reality in the future?

Final conclusion and evaluation statement

The structure of the work contains repeated subsections, which gives the impression of disorder. However, the extensive work associated with implementing two modelling procedures should be emphasised and appreciated. The suggestions mentioned above and criticisms do not change my positive opinion about this work. The doctoral dissertation meets all required criteria i.e.:
- it is an original solution to a scientific problem, which is the use of neural networks to predict the mechanical and electrical properties of concrete with the addition of CNT and CNF
- demonstrates the general theoretical knowledge of a PhD student in the discipline of civil engineering and transport.
- confirms the PhD student's ability to conduct independent research, also proved by numerous Author's publications in which she is an independent or the first Author.

The most important advantages of the reviewed dissertation of Ms Kekez include:

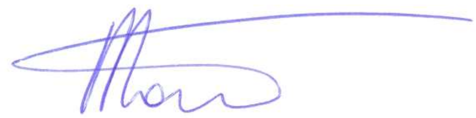
- the importance of the undertaken topic, including filling the research gap in the research topic of nanoparticles application in self-sensing concrete,
- a solid methodological framework, including the proper selection of research methods and their detailed description,
- awareness of the research limitations resulting from the method used (*Assumptions regarding numerical simulations*) and lack of information about the experiment in the available literature (*Assumptions regarding experimental work*),
- very high transparency of work and orderly scientific argument,
- critical approach to the obtained results of simulations,
- reliable study of the obtained results and documentation of results (appendices),
- the ability to formulate scientific conclusions.

Summing up, I can state that the reviewed doctoral dissertation meets the requirements of The Act of July 20, 2018, Higher Education Law and Science (with later amendments). The comprehensive experimental program conducted by the Candidate and the diversity of the research tools significantly expanded the Candidate's research competencies, enriching her research skills.

Ms Sofija Kekez, the Author of the thesis entitled: "Prediction of the mechanical and electrical properties of cementitious composites using artificial neural networks", submitted to the

Faculty of Civil Engineering and Transportation of the Silesian University of Technology, proved to have the ability to conduct scientific research. The presented doctoral dissertation constitutes an original solution to a scientific problem solved thanks to the Candidate's general theoretical knowledge in the discipline of civil engineering and transport. Taking the above into account, it fully meets the requirements of the Act. Therefore, I am applying for admission to public defence.

Respectfully,



Place: Cracow
Date: 08.09.2022

Izabela Hager, PhD, DSc, Eng.
Professor of Cracow University of Technology
Chair of Building Material Engineering
Cracow University of Technology
Warszawska 24, 31-155 Cracow, Poland
Tel: +48 605 030 832