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Opponent's review of the Doctoral Thesis

Candidate Christoph Pohl

Title of the doctoral thesis Numerical Modelling of Moisture Transport in Concrete under High Temperatures

Study Programme Civil Engineering (Branch of study: Physical and Material Engineering)

Tutor Doc. Ing. Vít Šmilauer, Ph.D., DSc. (Doctoral thesis co-tutor: Dr.-Ing. Jörg F. Unger)

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Topicality of the doctoral thesis theme

Commentary: The topics covered in the doctoral thesis fall perfectly within the field of civil engineering and in particular in the field of physics and materials engineering. Even if the main topic addressed has been studied by many researchers over the years, the problem of the concrete structures' behavior at high temperatures (e.g. during a fire) is still of great importance and many aspects have yet to be analyzed

☒ excellent	☐ above average	☐ average	☐ below average	☐ poor

Fulfilment of the doctoral thesis objectives

Commentary: the goals of the thesis, described very clearly at the beginning of the work, are fulfilled.

☐ excellent	☒ above average	☐ average	☐ below average	☐ poor

Research methods and procedures

Commentary: The research methods and procedures adopted are very good from both scientific and code-development points of view. A very detailed description of the most used numerical models available in the literature is presented with a precise analysis of their strengths and weaknesses. This part of the work is presented in a clear, systematic, and well-organized manner.

In particular, problems such as the choice of independent variables and balance equations, to be used in the formulation of the model, are discussed in depth. The choice and form of the constitutive laws are also described in detail.

On the other hand, in this part, there are some limits in the knowledge of the thermodynamics of multiphase porous materials and in the formulation of the models obtained starting from the micro-scale and applying averaging techniques.

The same approach was adopted for chapters 5 and 6 of the thesis. Also in this case the methodology used is more than good, the problem and the results obtained are presented clearly and properly discussed.

☐ excellent	☒ above average	☐ average	☐ below average	☐ poor

Results of the doctoral thesis – dissertant's concrete achievements

Commentary: The first part of the thesis is essentially dedicated to a review of what is available in the literature in the context of numerical modeling of concrete as a multiphase porous material. I appreciated this part because it is presented clearly and systematically. In this part of the work, the candidate shows remarkable skills in analysis.

However, the proposed model is very similar to what has been done in the past by other researchers and does not present truly innovative features apart from having explicitly treated the mass balance equation of the solid phase and taking porosity as the corresponding independent variable. The candidate highlighted the advantages of this approach compared to what was done in the formulation of other models. For example, it is no longer necessary to find a constitutive law for porosity and the solid skeleton mass balance is not violated (even if with a different approach it is sufficient to calculate the density of the solid phase properly during the computations). However, even the approach presented in the thesis shows some limitations, first of all adding an equation and an additional DOF to the model.

Anyway, the numerical implementation of such a kind of complex model is never trivial and the work done in this sense is very good.

The part of the thesis in chapters 5 and 6 is the natural complement of the model development. Chapter 5 shows the results related to the calibration and validation of the numerical model. In chapter 6 a detailed and very interesting analysis of uncertainty quantification together with the results of a sensitivity analysis of the main parameters are reported and discussed.

The results obtained are relevant in the context of the behavior of the material.

☐ excellent	☐ above average	☒ average	☐ below average	☐ poor

Importance for practice and for development within a branch of science

Commentary: As already pointed out, the topics treated in this thesis are of importance in civil engineering and in particular in the physics of building materials. For a real application to practical problems in civil engineering, the model should include a new part for the simulation of the mechanical behavior of the material and possibly of concrete structures. But I suppose this kind of development can be done in the next future (in the framework of another Ph.D. thesis).

☐ excellent	☐ above average	☒ average	☐ below average	☐ poor

Formal layout of the doctoral thesis and the level of language used

Commentary: from this point of view the work is excellent

☒ excellent	☐ above average	☐ average	☐ below average	☐ poor

Evaluation of author´s plagiarism

As far as I can see, there is no plagiarism (or self-plagiarism) by the author. He has cited all works needed.

Remarks

In this section, some remarks/questions are listed (to be addressed during the defense of the thesis).

Two comparisons with experimental test results are used for the calibration and validation of the numerical model. The first case (calibration) corresponds to a cylinder subjected to slow heating up to a target temperature of 300 ° C. The main aim is to measure the water content through X-ray Computer Tomography, plus the temperatures using a series of thermocouples. I understand that it is not easy to set and perform such a kind of test for a large number of specimens. Nonetheless, a single test for calibrating the constitutive relationships used in the model or to validate the model itself seems not sufficient. It would be better to use different heating profiles and target temperatures. Moreover, subsection 5.2 shows only graphs with the distribution in space of the relevant physical qualities (at different time instants). Some graphs showing the evolution of these physical quantities in time or in the domain of temperature (for some selected points) could be useful to better understand the behavior of the multiphase system. For this case no pressure measurements are available.

The experimental test used for the validation of the model consists of a column subjected to heating according to an ISO-Fire profile (subsection 5.3). In this part, the comparison of the experimental-numerical results is done in terms of temperature and pressure. Again only distributions in space are shown.

In all the cases shown in chapter 5, the boundary conditions are not described. For the case of the cylinder, we can suppose that they are of Dirichlet-type for the temperature (but for the mass exchange?). In the case of the heated column, there is no description of BCs. For instance: what is the heat exchange coefficient? There is also a radiative part of the heat supply? What is the mass exchange coefficient between the surface of the column and the environment? Fig. 5.9 seems without any description.

As far as the solid skeleton mass balance equation and the porosity as an independent variable are concerned, I am wondering if it is possible to show the evolution of the porosity in the domain of temperature in some selected points and then compare this evolution with the results of lab tests measuring the porosity (as a function of temperature)

The comparison shown in Fig. 5.7 is not completely clear to me. Fig. 5.6 seems to show the water mass loss strictly due to the hydration process (obtained by means of different approaches). For this purpose using the original formulation of the dehydration law is enough. But in Fig. 5.7, if I understand correctly, the results are related to the global water mass loss and they are obtained using the dehydration laws taken from different models (Tenchev, Dal Pont, etc.), but introduced into the model proposed in this thesis. The risk here is to have some inconsistency. Furthermore, some graphs with the evolution in time (and temperature) of the water mass loss in some selected points would help for a better understanding.

The part of the work related to the numerical implementation of the model is described very shortly. I understand that classical numerical techniques were used for this purpose, but most of the thesis is dedicated to the model as well as the title refers directly to numerical modeling. A more detailed description of the numerical implementation would have been needed. For instance: the set of governing equations is solved with a monolithic approach or with a partitioned (or staggered) approach? How the boundary conditions are passed from one part to another in case of a partitioned solution scheme is adopted? What are the convergence criteria and the stabilization techniques used?

Final assessment of the doctoral thesis

I appreciated this work.

In my opinion, and taking into account the grades in the various points, the final assessment of the present doctoral thesis is “above average”.

Following a successful defence of the doctoral thesis I recommend the granting of the Ph.D. degree		
	yes ☒	***no*** ☐

Date: 30/05/2022

Opponent's signature: .....