



Opponent's review of the Doctoral Thesis

Candidate: Michal Hlobil

Title of the doctoral thesis: Micromechanical analysis of blended cement-based composites

Branch of study: Physical and Material Engineering

Tutor: Dr. Vít Šmilauer (CTU in Prague) and Dr. Bernhard Pichler (TU Wien)

Opponent: Dr. Jan Zeman

e-mail: jan.zeman@fsv.cvut.cz

Topicality of the doctoral thesis theme

Commentary:

The submitted Ph.D. thesis focuses on time-dependent mechanical properties of cement-based composites, in which Portland cements are partially substituted with supplementary cementitious materials. The blending reduces the production costs and CO₂ emission, but also impacts the hydration kinetics and the hardening behavior of blended cement composites. Because these phenomena are still not well-understood, the development of their predictive models is clearly of a high scientific and industrial interest. This claim is further supported by the fact that the Ph.D. contract of Michal Hlobil have been fully funded by the industrial-academic research consortium NANOCEM.

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Fulfilment of the doctoral thesis objectives

Commentary:

The main objectives of the thesis are stated on page 4 and encompass (i) development of predictive models for compressive and tensile strength evolution, (ii) identification of main parameters governing compressive and tensile strengths, and (iii) validation of the models against data in the open literature supplemented with new experiments. Without a doubt, all these challenging objectives were met.

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Research methods and procedures

Commentary:

Research methods adopted by the candidate combine multi-scale (i) continuum micromechanics or (ii) numerical homogenization of heterogeneous materials with (iii) advanced techniques of microstructural characterization and (iv) novel methods to test effective (=macro-scale) properties of cementitious composites. The modelling part, which falls within my research expertise, clearly extends the state-of-the-art in (computational) micromechanics of materials, particularly in Chapter 5 dealing with up-scaling of the fracture energy.

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Results of the doctoral thesis – dissertant’s concrete achievements

Commentary: The following results constitute, in my opinion, the most significant contributions of the thesis:

- (i) CemBase -- a newly established database containing microstructural data and results of mechanical experiments, which collects data from about 300 pastes and 100 mortars based on blended and non-blended cements,
- (ii) novel experimental procedure for the determination of elastic modulus of cement pastes, which shows highly reproducible results (e.g., data scatter is smaller than for ultrasonic techniques),
- (iii) a novel hierarchical FE-based homogenization model based on the Griffith-Rankine damage model, which unveils the role of C-S-H gradient around cement grains,
- (iv) a refined version of an earlier model developed at TU Wien that applies also to the mortar scale and employs the Mohr-Coulomb criterion at the hydrate level. The model was successfully validated for conventional cementitious composites and difficulties with its extension towards blended cements were identified.
- (v) a novel hierarchical continuum micromechanics model to predict tensile behavior of cement-based composites, which was calibrated using data from direct tension tests by van Vliet and van Mier, and validated against independent three-point bending tests.

Of course, the results of this range cannot be achieved by a single person alone. The specific role of the Ph.D. candidate is clearly explained on pages 5--10, from which it follows that he significantly contributed to all results.

It is also worth noting that each of these achievements would provide a sufficient basis for a separate Ph.D. thesis (at least at the Czech Technical University in Prague). In addition, two chapters have already been published in peer-reviewed journals, which further highlights the quality and quantity of the achieved results.

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Importance for practice and for development within a branch of science

Commentary: The scientific contributions of the thesis appear summarized in the previous section.

I see the practical impact of the thesis in the development of validated models, based on minimalistic assumptions, which will contribute to more rational design of blended cement composites. Because of the involvement of the NANOCEM consortium, I am convinced that these outcomes are of a direct industrial interest.

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

Commentary: The thesis is clearly organized, carefully typeset, and written in excellent English.

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Remarks

During an oral defence, the Ph.D. candidate is kindly asked to address the following questions/remarks:

1. I agree with the author that one of the most useful outcomes of the thesis is the establishment of “CemBase”. However, I am missing more details on the main features of the database and its functionality. Do you plan to release the database as an open-source repository?

2. Data collected in Figure 1.7 on page 28, obtained with the ultrasonic wave technique, suggest that the scatter of the dynamic Young moduli of ordinary Portland cement pastes is substantially higher than for blended cements. Do you have an explanation for this phenomenon?

3. Figure 2.18 on page 59 shows significant variations of chemical affinity with increasing hydration degree. What is the reason for this behaviour? And how do your results compare to other studies available in the literature?
4. Does the model developed in Chapter 4 account for the presence of an interfacial transition zone around sand particles at the mortar level (e.g. Figure 4.1)? If this is not the case, please justify this modeling assumption.
5. For the same model, could you please estimate how the model predictions would change if (i) the von-Mises criterion is adopted instead of the Mohr-Coulomb criterion (Eq. (4.6)) and/or if (ii) the mean hydrate stresses are adopted instead of the quadratic averages?
6. If I understood it correctly, on pages 153 and 154 you claim that the covered sphere model share similar features with fractal size effect theories by Carpinteri and co-workers. Can you elaborate this connection in more details?

Final assessment of the doctoral thesis

In conclusion, this is an excellent Ph.D. thesis which significantly advances the state-of-the art in analytical and computational modeling of advanced cement-based composites. By successfully contributing to such challenging topic, Michal Hlobil has demonstrated his notable research skills in different disciplines of engineering mechanics of materials. It is therefore my pleasure to approve the thesis for an oral defence.

Following a successful defence of the doctoral thesis I recommend the granting of the Ph.D. degree

yes

no

Date: 2 October 2016

Opponent's signature:.....