

Numerical benchmark campaign of COST Action TU1404 – microstructural modelling

Supplementary material

Model 6 - Micromechanical numerical model

Mateusz Wyrzykowski¹, Julien Sanahuja², Laurent Charpin², Markus Königsberger³, Christian Hellmich³, Bernhard Pichler³, Luca Valentini⁴, Túlio Honório⁵, Vit Smilauer^{6*}, Karolina Hajkova⁶, Guang Ye⁷, Peng Gao⁷, Cyrille Dunant⁸, Adrien Hilaire⁹, Shashank Bishnoi¹⁰, Miguel Azenha¹¹

¹ Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland

² EDF, R&D MMC, France

³ TU Wien, Austria

⁴ University of Padua, Italy

⁵ Université Paris-Est, Laboratoire Navier (UMR 8205), CNRS, ENPC, IFSTTAR, France

⁶ Czech Technical University in Prague, Czech Republic

⁷ TU Delft, The Netherlands

⁸ Department of Engineering, University of Cambridge, UK

⁹ EPFL, Lausanne, Switzerland

¹⁰ IIT Delhi, India

¹¹ ISISE, University of Minho, Portugal

Received: 5 December 2017 / Accepted: 25 December 2017 / Published online: 30 December 2017

© The Author(s) 2017. This article is published with open access and licensed under a Creative Commons Attribution 4.0 International License.

1 Introduction

In this document the input data for the *Model 6 - Micromechanical numerical model* used in the numerical benchmark [1] is presented as a supplementary material.

2 Input data - model 6

Hydration model: CEMHYD3D

Resolution: 1 $\mu\text{m}/\text{voxel}$

RVE size: 100 x 100 x 100 μm

PSD of cement: Indirectly through Blaine surface area

Clinker mineralogy: Entered from experimental values

Min particle diameter: 1 μm

Max particle diameter: 46 μm

Model for elasticity:

Formulation: Continuum micromechanics

Multiscale approach: Yes

Use of volume fractions: Yes - from percolated 3D microstructure

Intrinsic elastic modulus for C-S-H (LD): 21.7 GPa

Intrinsic elastic moduli for other hydrates: 22.4-42.3 GPa

Intrinsic elastic modulus for clinker minerals (without gypsum): 125-145 GPa

Model for strength:

Formulation: Numerical micromechanics

Multiscale approach: Yes

Weakest solid phase causing failure: C-S-H globule

Failure law: Softening of C-S-H globule.

References

- [1] M. Wyrzykowski, et al., Numerical benchmark campaign of COST Action TU1404 – microstructural modelling. RILEM Technical Letters (2017) 2: 99-107. <http://dx.doi.org/10.21809/rilemtechlett.2017.44>

* Corresponding author (this supplementary material): Vit Smilauer, E-mail: vit.smilauer@fsv.cvut.cz