RILEM Technical Letters (2017) 2: 99-107
DOI: http://dx.doi.org/10.21809/rilemtechlett.2017.44 Supplementary material

Numerical benchmark campaign of COST Action TU1404 – microstructural modelling

Supplementary material
Model 4 - Micromechanical analytical model

Mateusz Wyrzykowski[1], Julien Sanahuja[2], Laurent Charpin[2], Markus Königsberger[3], Christian Hellmich[3], Bernhard Pichler[3], Luca Valentini[4], Túlio Honório[5*], Vit Smilauer[6], Karolina Hajkova[6], Guang Ye[7], Peng Gao[7], Cyrille Dunant[8], Adrien Hilaire[9], Shashank Bishnoi[10], Miguel Azenha[11]

[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

1 Introduction

In this document the input data for model 4 - *micromechanical analytical model* used in the numerical benchmark [1] is presented as a supplementary material.

2 Input data - model 4

PSD was explicitly taken into account in the scenario following hydration kinetics model presented in [2].

From the oxide composition o cement provided, the contents of clinker minerals are obtained through Bogue equations.

Hydration balance equation of Tennis and Jennings [3] are used to represent hydration product assembly.

The multiscale nature of cement-based materials is depicted in the Figure 1.

The elastic properties of the phases at the cement paste scale are given in the Table 1.

* Corresponding author (this supplementary material): Túlio Honório, E-mail: tulio.honorio-de-faria@enpc.fr

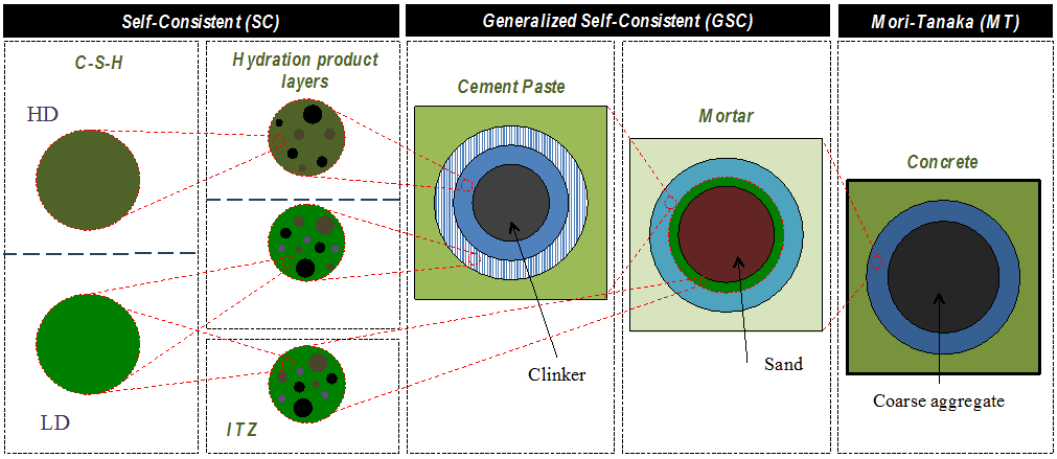

Figure 1 Representation of the multiscale nature of cement-based materials as in [4].

Table 1 Elastic properties of the different phases as in [5].

	Clinker	C-S-H		CH	AFt	AFm	$C_3(A,F)H_6$	C_4AH_{13}	Gypsum	Sand
		LD	HD							
E [GPa]	140	21.7	29.4	38	22.4	42.3	22.4	25	45.7	74.5
v	0.3	0.24	0.24	0.305	0.25	0.324	0.25	0.25	0.33	0.2
Ref.	[6]	[7]	[7]	[8]	[9]	[9]	[10]	[10]	[10]	[11]

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

[2] T. Honorio, B. Bary, F. Benboudjema, S. Poyet, Modeling hydration kinetics based on boundary nucleation and space-filling growth in a fixed confined zone. Cem Concr Res (2016) 83: 31-44. https://doi.org/10.1016/j.cemconres.2016.01.012

[3] P.D. Tennis, H.M. Jennings, A model for two types of calcium silicate hydrate in the microstructure of Portland cement pastes. Cem Concr Res (2000) 30: 855-863. https://doi.org/10.1016/S0008-8846(00)00257-X

[4] T. Honorio, B. Bary, F. Benboudjema, Thermal properties of cement-based materials: multiscale estimations at early-age. Cem Concr Compos (2017, submitted).

[5] T. Honorio, B. Bary, F. Benboudjema, Multiscale estimation of ageing viscoelastic properties of cement-based materials: A combined analytical and numerical approach to estimate the behaviour at early age. Cem Concr Res (2016) 85: 137-155. https://doi.org/10.1016/j.cemconres.2016.03.010

[6] K. Velez, et al., Determination by nanoindentation of elastic modulus and hardness of pure constituents of Portland cement clinker. Cem Concr Res (2001) 31: 555-561. https://doi.org/10.1016/S0008-8846(00)00505-6

[7] O. Bernard, F.-J. Ulm, E. Lemarchand, A multiscale micromechanics-hydration model for the early-age elastic properties of cement-based materials. Cem Concr Res (2003) 33: 1293-1309. https://doi.org/10.1016/S0008-8846(03)00039-5

[8] P.J.M. Monteiro, C.T. Chang, The elastic moduli of calcium hydroxide. Cem Concr Res (1995) 25: 1605-1609. https://doi.org/10.1016/0008-8846(95)00154-9

[9] S. Kamali, Comportement et simulation des matériaux cimentaires en environnement agressifs: lixiviation et température. Cachan, Ecole normale supérieure, 2003.

[10] C.J. Haecker, et al., Modeling the linear elastic properties of Portland cement paste. Cem Concr Res (2005) 35: 1948-1960. https://doi.org/10.1016/j.cemconres.2005.05.001

[11] E. Stora, Multi-scale modelling and simulations of the chemo-mechanical behavior of degraded cement-based materials. Université Paris-Est, 2007.