XVII International Conference on Computational Plasticity, COMPLAS 2023
September 5-7, 2023, Barcelona, Spain

MULTISCALE MODELING OF CONCRETE WITH NANO-INGREDIENTS

MARIUSZ POŃSKI*, IWONA POKORSKA*
AND TADEUSZ BURCZYŃSKI*

* Institute of Fundamental Technological Research, Polish Academy of Sciences
A. Pawińskiego 5b, 02-106 Warsaw, Poland
mponski@ippt.pan.pl,ipokorsk@ippt.pan.pl, tburczynski@ippt.pan.pl
https://www.ippt.pan.pl/en/

ABSTRACT

Different kind of ingredients can be located in concrete structures in order to improve their mechanical and thermal features. The paper contains the case when nano-ingredients in the form of petals of graphene or nanotubes are taken into account. Because of the fact that concrete is heterogeneous medium and ingredients have nano-scale the multiscale modelling is proposed to solve the problem [1]. The key problem is creation of a representative unit cell which contains representative inhomogeneities on the micro level and influence of nano-ingredients on local substructure. To solve this problem multistage computations have to be performed [2]. At the first stage molecular approach to nanoscale is applied using LAMMPS software. Elastic properties from the first stage solution are used to obtain microscale solution which consists of cement paste incorporating a combination of C-S-H, capillary pores and other hydration products including Portlandite (Calcium hydroxide (CH)), Ettringite, and un-hydrated cement grains. This procedure is repeated until the macroscale (cement paste in combination with aggregate) mechanical properties of representative volume element is computed. Due to its advantages in modelling the microstructural development of realistic Portland cements (including particle sizes), and the ability to incorporate customised hydration behaviour from isothermal calorimetry, the VCCTL software (Virtual Cement and Concrete Testing Laboratory) is selected to simulate the microstructural development of a cement. The multiscale micro-macro problem is solved using the homogenization approach. Computer implementation of the established approach and examination of accepted terms are discussed. Numerical tests and examples are presented.

REFERENCES

[1] Burczyński T., Pietrzyk M., Kuś W., Madej Ł., Mrozek A., Rauh Ł., *Multiscale Modelling and Optimisation of Materials and Structures*, Willey 2022.

[2] Zhang, H., Xu, Y., Gan, Y., Chang, Z., Schlangen, E., & Šavija, B., *Microstructure informed micromechanical modelling of hydrated cement paste: Techniques and challenges*. Construction and Building Materials, 251, 118983, 2020.