An upscaling method for predicting the behavior of concrete structures under brine attack

Gili Lifshitz Sherzer, Department of Structural Engineering, Ben-Gurion University of the Negev, Beer-Sheva, Israel, gili.lifshitz@gmail.com

Konstantin Kovar, Faculty of Civil and Environmental Engineering, Technion University - Israel Institute of Technology, Haifa, Israel, cvrkost@technion.ac.il

Guang Ye, Microlab/Section of Materials and Environment, Faculty of Civil Engineering and Geosciences, Delft University of Technology, The Netherlands, G.Ye@tudelft.nl

Erik Schlangen, Microlab/Section of Materials and Environment, Faculty of Civil Engineering and Geosciences, Delft University of Technology, The Netherlands, Erik.Schlangen@tudelft.nl

Erez Gal, Department of Structural Engineering, Ben-Gurion University of the Negev, Beer-Sheva, Israel, erezgal@bgu.ac.il

ABSTRACT

Concrete contains layers of complexity and considered as a heterogeneous material, thus assessing the concrete response through multiscale analysis, requires a development of up scaling approach. Concrete being a composite material that contain more than two finely mixed constituents, results a complex modelling procedure. The multiscale approach is achieved by retrieving the macroscopic properties from the cement and mortar scales. The overarching goal of this paper is to apply the Lattice model developed in Delft in order to obtain the compression numerical parameters, required for the evaluation of the Lattice Discrete Particle Model (LDPM) Pore Collapse and Material Compaction parameters. This aim was successfully achieved in the Microlab/Section of Materials and Geosciences, under the co-workers of Prof. Klaas van Breugel, Prof. Erik Schlangen and Dr. Ye Guang. Towards this goal, the specific scientific objective of this paper is to formulate, calibrate, and validate multi-scale models based on the homogenization of a recently developed discrete meso-scale model known as the Lattice Discrete Particle Model (LDPM). Furthermore, in this paper, a multiscale analysis procedure is proposed for modelling concrete structures, in which material properties at the macro scale are retrieved from the components and their geometrical distribution in the micro structure. In addition, we implemented the up-scaling method in order to analyses the stability, longevity, and durability of a concrete wall located at the Dead Sea. The models were calibrated and validated using experimental results and the results looks promising as microscopic calibrated parameters were able to predict accurate macroscopic results.

INTRODUCTION

Predicting the behavior of concrete structures is increasingly difficult. Usually the mechanical behavior of concrete is macroscopically modeled via plastic constitutive relations [1-3]. These macroscopic models are characterized by the large number of parameters needed to be calibrated in order to analyze the complex behavior of the concrete at the different stages of loading and at the different damage modes. Using these macroscopic models is complicated due to the fact that the concrete has a variety of microstructures and actually has no distinctive microstructure. The concrete mix design has to meet new standards technology of high-performance solutions that includes: addition of fibers made up from different materials; aggregate-size distribution, shape and type; water to cement ratio etc. The use of multi-scale analysis evidently is the appropriate way to model the behavior of concrete structures by coupling between the concrete micro-structures and its macroscopic properties needed to analyze a structure [4-16]. There are researches that deals with the influence of multi-scale micro structure on concrete thus, enabling a description of the heterogeneous character of the cement paste and evaluation of its mechanical properties according to its hydration processes [17-21].

In this research we are evaluating, calibrating and validating the mechanical parameters of the LDPM [22, 23] based on the cement paste and mortar scales. In order to consider all the scales up to the LDPM model, it is necessary to develop a methodology to amalgamate the information generated from each of the cement paste, mortar, and concrete scales. The evaluation of the mechanical parameters for the LDPM is based on the cement paste and mortar scales. In order to consider all the scales up to the LDPM model, it is necessary to develop a methodology to amalgamate the information generated from each of the cement paste, mortar, and concrete scales. We propose that this can be achieved by defining parameters for input into the LDPM model that correctly describe each failure mode based on the lower levels. These will be implemented based on the following models: HYMOSTRUC [24, 25], lattice model [26] of the hydrated cement, and models for mortar (Anm [27] material and lattice [26] models).

In addition, we implement this approach to analyze a concrete wall. This wall is embedded in the ground under the Dead Sea and exposed to aggressive environmental conditions. The wall stability is severely endangered due to the exposure to these conditions, therefore the durability of the wall's service life, designed to last for a period of 40 years, needs to be simulated. The simulations for this purpose were up-scaled up to the mortar-a4 scale.

METHODOLOGY

The upscaling methodological approach for evaluating the LDPM parameters was explained in detail in the previous articles [28, 29], while in this section we focused on predicting the compressive strength of the wall at the age of 40 years' service life. This section explains simplistically step by step the following process, the first step includes defining the equivalent w/c ratio that represent the effect of the sulfate attack on the wall, leading to loss of concrete strength. The second step includes variable microstructures, obtained from HYMOSTRUC3D simulation using the equivalent w/c ratio defined for different ages of the wall exposed to brine. Finally, the third step includes mechanical numerical simulations performed by the lattice model.

The lattice model simulations performed on the cement paste scale has two purposes: 1. To simulate compressive tests under completely confined uniaxial compression loads, in order to select the appropriate unit cell size that will include the Pore Collapse phenomenon under confined conditions and partially confined uniaxial compression loads equivalent to the ground pressure, to study the stability of the wall over a period of 40 years; 2. To simulate tension tests in order to upscale the mechanical properties as an input for the higher scale, mortar-s. Then using the mechanical properties of the cement paste as an input for simulating tension test on mortar-s scale, in order to obtain the mechanical properties of the concrete scale represented by the mortar-a4 scale. The last step was the unconfined compression simulation tests, that was performed on the concrete scale at three different ages of the wall exposed to brine: 28 d to calibrate mechanical interface properties; 57 d to validate the model by comparing the simulation results with the experimental results, and; 40 y to predict the stability and durability of the wall under unconfined conditions. It should be noted that these ages, were selected in order to be compatible with unconfined uniaxial compression

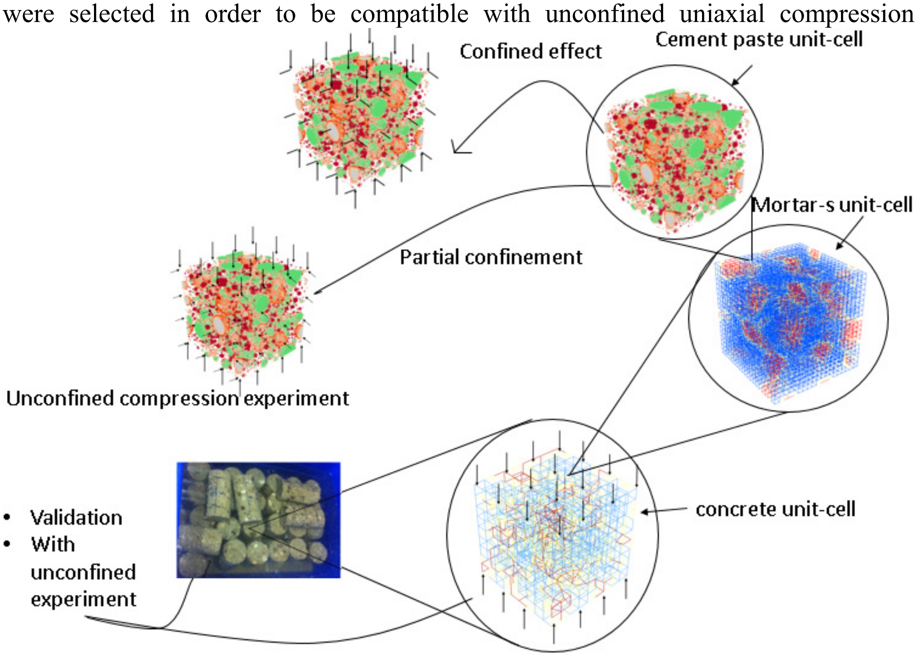

Figure 1: Multiscale approach for concrete wall embedded in the ground under the Dead Sea.

experiments, conducted on specimens drilled from the wall. A flowchart describing the methodology is presented in Figure 1.

Microstructure Modelling of the Cement Paste

Input parameters

In order to account the briny environmental conditions on the behavior of concrete, we defined an effective *w/c* ratio at certain time points representing different concrete ages. We developed a method that relates between the chemical reaction effected by the brine and the material degradation, by an increasing effective water-cement ratio w/c that represent the grow of the porosity and effect the loss of the material strength. For this purpose, we adopted the approach of [30] that defines the w/c from the concrete compressive strength, as presented in Equation 1. This approach is conceded as the most popular/accepted method to represent the strength of the concrete as a function of the w/c ratio

(1) $$\sigma = \frac{A}{B^{\omega}}$$

where A and B are constants and ω is the effective *w/c* ratio. The constants were defined, by curve fitting between curve CEM 42.5 as appears in [30] and Equation 1. For example, for the presented simulation, the cement type is CEM 42.5, where A=125.4 and B=9.29.

The proper effective *w/c* ratios needed for the simulations were achived by the experiments results of unconfined compressive strength performed at different concrete ages, as presented in Table 1. The compressive strength from the experiments was used in Equation (1), in order to obtain the effective *w/c* ratio (see Table 1):

Table 1: Strength, time and effective w/c data.

σ (MPa)	Time (day)	w/c
6.21	3	1.35
3.28	28	1.63
2.92	57	1.69
1.6	120	1.96

To evaluate the microstructure, the HYMOSTRUC3 model, was used. The simulations were performed on the material mix design, of a wall located at the Dead Sea, used as a case study. The microstructure specimen size of 100 μm × 100 μm × 100 μm, was selected and the effective *w/c* ratio from Table 1 was used for the simulations.

For the analyses of the wall stably at 40 years (service life), the effective w/c ratio needs to be defined. This simulated analysis over a 40-year period was accomplished by using the microstructure at the age of 317 d, at which point the cement products have reached approximately 99% of their hydration. The effective *w/c* ratio for the 40 y was evaluated using the following logarithmic Equation (2), based on the experiment data from Table 1 and demonstrated at Figure 2.

(2) $$w/c = 0.1507 \cdot ln(time(d)) + 1.1571$$

The effective *w/c* ratio at 40-year was found to be 2.6.

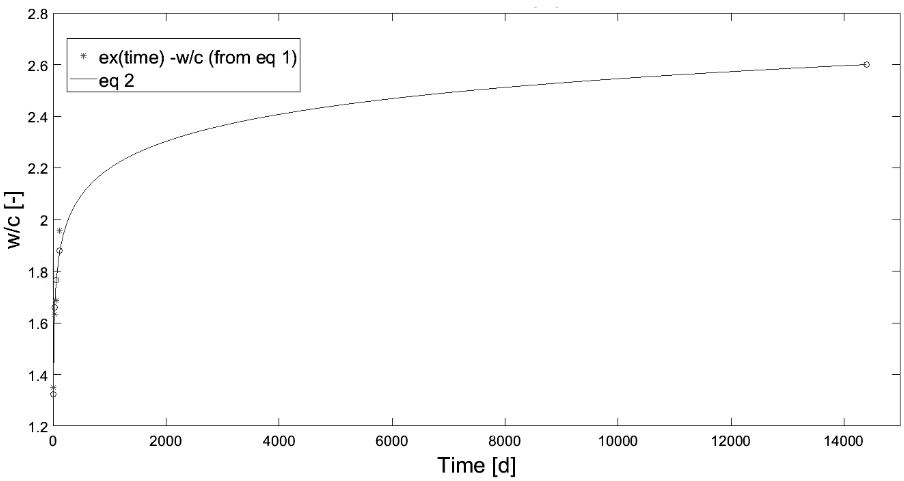

Figure 2: Effective w/c ratio at 40 y

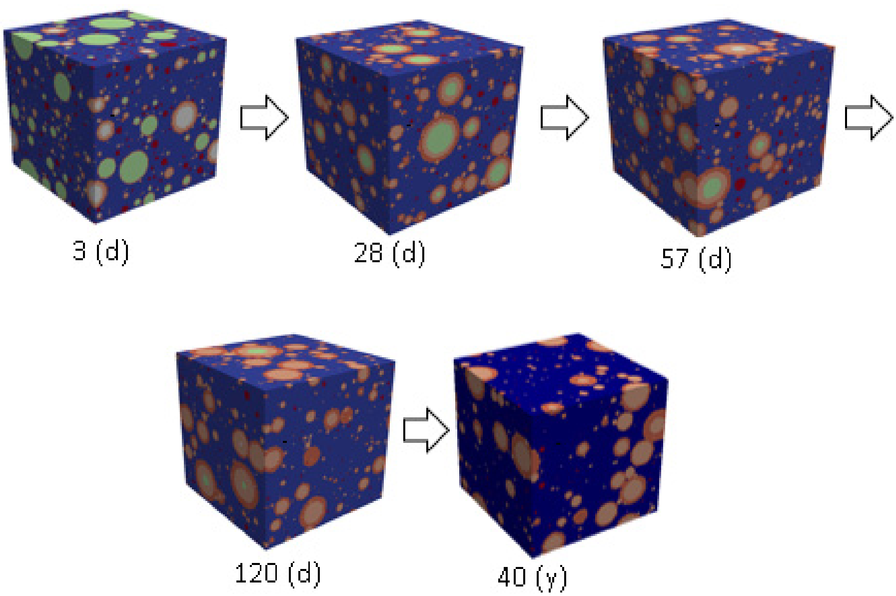

Figure 3: Microstructure results

OUTPUT RESULTS

The microstructures at ages of 3 d, 28 d, 120 d and 40 y are presented in Figure 3.

CONCLUSION

The essential part of this study was an expression of microstructural changes resulting in the increase of the material porosity via the "effective w/c ratio", that represent the degradation of the material due to the brine attack. The stability of the wall is endangered, as a result of continuous material erosion. Thus, a case study of the wall's strength under brine attack was performed. The briny environment, conditions were taken into account in our proposed approach by determining an equivalent w/c ratio for different porosities corresponding to the duration exposer to brine. In addition, the confinement conditions, due to the ground presser was considered.

ACKNOWLEDGEMENTS

This research was supported by the Israel Ministry of Science, Technology and Space, Government of Israel; COST Action TU1404; and Nesher-Israel Cement Enterprises.

REFERENCES

[1] Drucker, D. C., & Prager, W. (1952). Soil mechanics and plastic analysis or limit design. *Quarterly of applied mathematics, 10*(2), pp. 157-165.

[2] Riedel, W., Thoma, K., Hiermaier, S., & Schmolinske, E. (1999). *Penetration of reinforced concrete by BETA-B-500 numerical analysis using a new macroscopic concrete model for hydrocodes.* Proceedings of the 9th International Symposium on the Effects of Munitions with Structures.

[3] Shin, K.-J., Lee, K.-M., & Chang, S.-P. (2008). Numerical modeling for cyclic crack bridging behavior of fiber reinforced cementitious composites. *Structural Engineering and Mechanics, 30*(2), pp. 147-164.

[4] ,Kabele, P. (2007). Multiscale framework for modeling of fracture in high performance fiber reinforced cementitious composites. *Engineering Fracture Mechanics, 74*(1-2), pp. 194-209.

[5] Li, V. C. (1993). From Micromechanics to Structural Engineering. *Doboku Gakkai Ronbunshu, 1993*(471), pp. 1-12.

[6] Lange-Kornbak, D., & Karihaloo, B. (1998). Design of fiber-reinforced DSP mixes for minimum brittleness. *Advanced cement based materials, 7*(3-4), pp. 89-101.

[7] Cusatis, G., Bazant, Z. P., & Cedolin, L. (2001). *3D Lattice model for dynamic simulations of creep, fracturing and rate effect in concrete.* Proceedings of the 6th International Conference on Cambridge, Cambridge, MA, USA.

[8] Cusatis, G., Bažant, Z. P., & Cedolin, L. (2003). Confinement-shear lattice model for concrete damage in tension and compression: I. Theory. *Journal of Engineering Mechanics, 129*(12), pp. 1439-1448.

[9] Cusatis, G., Polli, M., & Cedolin, L. (2004). *Mesolevel analysis of fracture tests for concrete.* Fracture Mechanics of Concrete Structures, Proceedings of the Fifth International Conference on Fracture Mechanics of Concrete and Concrete Structures—FraMCoS-5, Vail Cascade Resort, Vail Colorado, Ia-FraMCos, USA.

[10] Cusatis, G., & Cedolin, L. (2007). Two-scale study of concrete fracturing behavior. *Engineering Fracture Mechanics, 74*(1-2), pp. 3-17.

[11] Cusatis, G., Bažant, Z. P., & Cedolin, L. (2006). Confinement-shear lattice CSL model for fracture propagation in concrete. *Computer methods in applied mechanics and engineering, 195*(52), pp. 7154-7171.

[12] Cusatis, G., Pelessone, D., & Mencarelli, A. (2011). Lattice discrete particle model (LDPM) for failure behavior of concrete. I: Theory. *Cement and Concrete composites, 33*(9), pp. 881-890.

[13] Cusatis, G., Pelessone, D., Mencarelli, A., & Baylot, J. T. (2007). *Simulation of reinforced concrete structures under blast and penetration through lattice discrete particle modeling.* ASME 2007 International Mechanical Engineering Congress and Exposition.

[14] Cusatis, G., Mencarelli, A., Pelessone, D., & Baylot, J. T. (2008). *Lattice discrete particle model (LDPM) for fracture dynamics and rate effect in concrete.* Structures Congress 2008: 18th Analysis and Computation Specialty Conference.

[15] Gal, E., Ganz, A., Hadad, L., & Kryvoruk, R. (2008). Development of a concrete unit cell. *International Journal for Multiscale Computational Engineering, 6*(5)

[16] Gal, E., Suday, E., & Waisman, H. (2013). Homogenization of materials having inclusions surrounded by layers modeled by the extended finite element method. *International Journal for Multiscale Computational Engineering, 11*(3)

[17] Qian, Z. (2012). Multiscale modeling of fracture processes in cementitious materials.

[18] Bentz, D. P., Garboczi, E. J., & Lagergren, E. S. (1998). Multi-scale microstructural modeling of concrete diffusivity: Identification of significant varibles. *Cement, Concrete and Aggregates, 20*(1), pp. 129-139.

[19] Bullard, J. W., & Garboczi, E. J. (2006). A model investigation of the influence of particle shape on portland cement hydration. *Cement and Concrete Research, 36*(6), pp. 1007-1015.

[20] Constantinides, G., & Ulm, F.-J. (2004). The effect of two types of CSH on the elasticity of cement-based materials: Results from nanoindentation and micromechanical modeling. *Cement and Concrete Research, 34*(1), pp. 67-80.

[21] Garboczi, E., & Berryman, J. (2000). New effective medium theory for the diffusivity or conductivity of a multi-scale concrete microstructural model. *Concrete Science and Engineering, 2*, p 8896.

[22] Cusatis, G., Pelessone, D., & Mencarelli, A. (2011). Lattice discrete particle model (LDPM) for failure behavior of concrete. I: Theory. *Cement and Concrete composites, 33*(9), pp. 881-890.

[23] Cusatis, G., Mencarelli, A., Pelessone, D., & Baylot, J. (2011). Lattice discrete particle model (LDPM) for failure behavior of concrete. II: Calibration and validation. *Cement and Concrete composites, 33*(9), pp. 891-905.
[24] Ye, G., Van Breugel, K., & Fraaij, A. (2003). Three-dimensional microstructure analysis of numerically simulated cementitious materials. *Cement and Concrete Research, 33*(2), pp. 215-222.
[25] Van Breugel, K. (1995). Numerical simulation of hydration and microstructural development in hardening cement-based materials (I) theory. *Cement and Concrete Research, 25*(2), pp. 319-331.
[26] Qian, Z., Schlangen, E., Ye, G., & Van Breugel, K. (2012). *Multiscale lattice fracture model for cement-based materials.* ICCM 2012: 4th International Conference on Computational Methods, Gold Coast, Australia, 25-28 November 2012.
[27] Qian, Z., Garboczi, E., Ye, G., & Schlangen, E. (2016). Anm: a geometrical model for the composite structure of mortar and concrete using real-shape particles. *Materials and Structures, 49*(1-2), pp. 149-158.
[28] Sherzer, G., Gao, P., Schlangen, E., Ye, G., & Gal, E. (2017). Upscaling Cement Paste Microstructure to Obtain the Fracture, Shear, and Elastic Concrete Mechanical LDPM Parameters. *Materials, 10*(3), p 242.
[29] Sherzer, G. L., Gal, E., Schlangen, E., & Ye, G. (2018). *Multi-scale modelling of the mechanics of concrete based on the cement paste properties.* Computational Modelling of Concrete Structures: Proceedings of the Conference on Computational Modelling of Concrete and Concrete Structures (EURO-C 2018), February 26-March 1, 2018, Bad Hofgastein, Austria.
[30] M. Rais, *Manual for Civil Engineers 1980*.