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Multi-scale Modelling of the Mechanics of Concrete Based on the Cement Paste Properties

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ABSTRACT: The mechanical response of concrete is complex and as other composite materials, multiscale modelling has the potential for modeling its macroscopic behavior. This paper presents an upscaling methodology for the modelling of the concrete mechanical properties. The suggested formulation starts from a known chemical and mechanical set of parameters of the cement paste, which are used to evaluate the mechanical properties of the LDPM (Lattice Discrete Particle Model) concrete mechanical parameters. The parameters are divided to groups, which are related to different damage modes such as: pore collapse and material compaction, cohesive behavior, and shear behavior. For each group of parameters, a set of microscopic simulations are performed to complete the up-scaling methodology.

INTRODUCTION

Concrete is a material that shows significant differences in the behavior of the stress-strain diagram under various combinations of loads. As concrete is considered as a composite material, the stress state within a specimen is strongly heterogeneous, even for homogeneous macroscopic loading situations. The concrete under tensional loads performs a softening behavior after the fracture strength is reached. Therefore, the specimen does not collapse instantaneously but the stress decreases gradually for increasing deformation. The softening behaver is strongly depended on the microstructure changes, for example change in the mineral composition, water to cement (w/c) ratio, change in the components of the elastic material stiffness, see also Z. Qian (2012). According to G. Hofstetter (1995), approximately at 60% of the maximum load, microcracks form through the Interface Transition Zone (ITZ) between aggregates and mortar matrix. By increasing the load, the interface cracks form through the mortar matrix and additional microcracks initiate within the mortar matrix. However, the damage of concrete under compression starts at very low strain-levels leads to failure in a progressive way, consequently the pre-critical crack growth is much larger than in tension.

For the behavior of concrete under high levels of confinement begins with initial peak point due to collapse of the material porous microstructure and followed by a hardening behavior due to closure of the pores. X. Vu et al. (2009) focus on the effects of the (w/c) ratio, entering the fresh concrete composition, on hardened concrete behavior under very high confinement. The finding of that work was that a drop-in (w/c) ratio pushes the confinement threshold higher, however beyond a critical mean stress, the limit state curve becomes independent of (w/c) ratio.

The damage of concrete under shear loads, appears as a mechanism induce tensile stresses in the concrete near the crack. Once the tensile strength of the concrete in these regions is reached, existing flexural cracks propagate in a diagonal direction or new cracks are created.

This paper deals with the development of a methodology for upscaling the cement scale response to obtain the mechanical parameters at the concrete scale. The evaluation of mechanical LDPM’s parameters was achieved from the lower scale models under different load combinations that is suitable to represent the failure mechanism of the parameters. In this paper, we achieved from the suggested upscaling method, the flowing parameters; two cohesive, one shear and six pore collapses under compaction, while two elastic and four remaining parameters were achieved by macroscopic calibration.

The suggested methodology is based on a multiscale analysis procedure, in which material properties at the macro scale are evaluated based on lower scales. The cement paste scale is characterized by cement products prior to and following the hydration process; the cement grain particle size range is 1–50 μm. For this scale, we suggest analysis using a lattice model Z. Qian *et al.* (2012). For the mortar-s scale including the cement paste as a matrix, sand as inclusion, and an (ITZ); the sand particle size range is 1.2–0.5 mm. For this scale, we suggest using the

Anm and lattice models Z. Qian et al. (2016), Z. Qian et al. (2012). The mortar-a4 scale includes the combination of mortar-s as a matrix, with aggregates smaller than 4 mm as inclusions and an interface layer between them; the aggregate size range is 2.36–4 mm. The designation mortar-a4 was given to emphasize the fact that the aggregates are smaller than 4 mm. For this scale, we suggest using the Anm and lattice models Z. Qian et al. (2016), Z. Qian et al. (2012). The concrete scale includes aggregates larger than 4 mm (and usually up to 20 mm) and mortar-a 4 as a matrix; we consider this scale to be the concrete scale. For this scale, we suggest using the LDPM.

METHODOLOGY OF RESEARCH

The upscaling suggested procedure bridges between the scales from the properties of the lower scales. Each LDPM parameters relate to a different failure modes and can therefore, be derived from a different set of simulations G. Cusatis, et al. (2011A, B) of the lower scales. The constitutive equations of the LDPM represent the mechanical behavior at the facets in which the mortar is located; therefore, it can be assumed that the facet failure modes can be characterized by a unit cell of the mortar, which includes aggregates smaller than 4 mm. As depicted in Figure 1 we assumed that the mortar-a4 scale is suitable to represent the unit cell of the facet, however to represent the failure criterion of the pore collapse mode, we assumed that it can be characterized by a unit cell of the cement paste, since only at that scale porosity is consider. The flowchart of the suggested methodology is depicts in Figure 2.

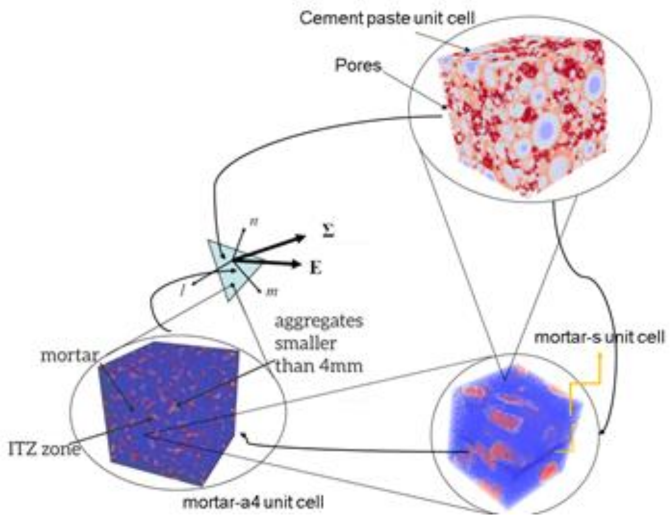

Figure 1. The LDPM facet and the lower scale unit cells

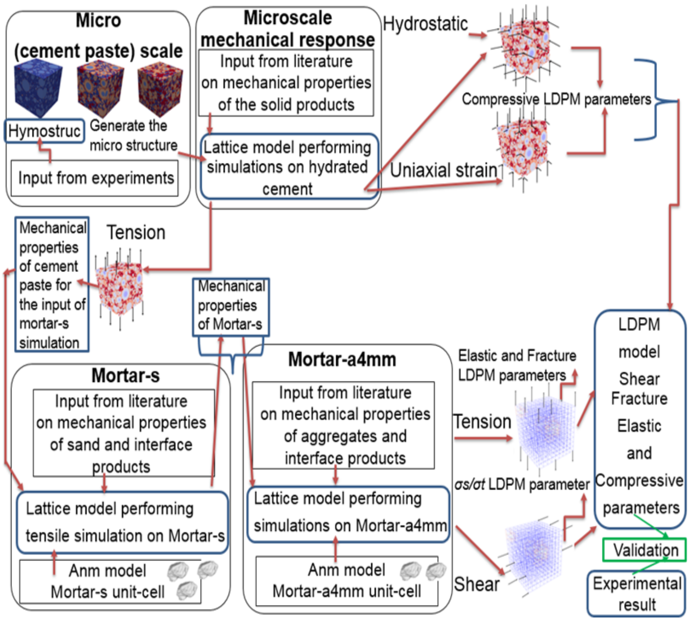

Figure 2. Flowchart of the suggested upscaling procedure.

For convenience, we divided the LDPM parameters (for more details see G. Cusatis et al. (2011), Z.P.; Bazant (1989)) to the following groups:

Elastic parameters

Two elastic parameters, which obtained at this stage of the research using macroscopic calibration:

1. E_0, the normal elastic modulus.
2. α the shear-normal coupling parameter.

Fracture Parameters

Two fracture parameters, which represent the tensile mode:

1. σ_t, tensile strength
2. l_t, modified characteristic length

These two parameters were achieved using the suggested methodology as depicted in Figure 2.

Pore collapse parameters

Six pore collapse and material compaction parameters, which represent the compression behavior:

1. σ_{co} the yielding compressive stress.
2. E_D/E_0 the densification ratio.
3. H_{co}/E_0 the initial hardening modulus ratio.
4. k_{co} the transitional strain ratio.
5. k_{c1} nonlinear evolution parameter.
6. k_{c2} nonlinear evolution parameter.

These two parameters were achieved using the suggested methodology as depicted in Figure 2.

Shear Parameters

Two shear parameters representing the interaction between shear and tensile behavior.

1. n_t, shear softening exponent parameter, at this stage of the research obtained using macroscopic calibration.
2. σ_s/σ_t is the shear-to-tensile strength ratio. These parameters were achieved using the suggested methodology as depicted in Figure 2.

RESULTS

For validation, we compare the numerical results obtained using the suggested methodology with experimental results (see Sherzer et al (2015)), as shown in Figure 3. Figure 3, shows a comparison of the longitudinal and transverse displacement components measured from uniaxial compression test of a 100mmx100mmx100mm concrete specimen. The input of the cement paste scale is given in Table 4 and 5. The Up-scaled LDPM parameters using the suggested methodology and the calibrated LDPM parameters are presented in Table 2 and Table 3 respectively, while the concrete mixture properties are presented in Table 1.

Table 1. Concrete Mix-design parameters

Parameters	units		units
	Kg/m^3	-	mm
C	391	-	-
w/c	-	0.567	-
a/c	-	2.2532	-
d_o	-	-	4
d_a	-	-	14
N_F	-	0.425	-

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Table 2. Up-scaled LDPM Parameters

Parameters	Calibrated		Up-scaled	
	MPa	-	MPa	-
σ_t	4.03	-	4.259	-
G_t	32.32	-	29.62	-
σ_s/σ_t	-	2.7	-	2.63
σ_{co}	70	-	81.09	-
Hco/E_0	0.4	-	0.35	-
K_{c0}	-	2	-	2.72
K_{c1}	-	1	-	1
K_{c2}	-	5	-	0.4975

Table 3. Calibrated LDPM parameters

Parameters	Calibrated	
	MPa	-
E_0	30150	-
α	-	0.38
n_t	-	0.5
μ_o	-	0.2
μ_∞	-	0
σ_{No}	-	600

Table 4. Chemical Properties of the Cement

Characteristic	Inputs Specification
Mineralogical composition (%)	C3S: 54.9, C2S: 19.1, C3A: 4, C4AF: 8.8
Chemical composition (%)	Al_2O_3: 6.41, SiO_2: 20.39, MgO: 1.08, CaO: 58.58, Fe_2O_3: 3.92, SO_3: 2.92, Na_2O: 0.22, K_2O: 0.44
Minimum particle diameter	1 μm
Cement fineness (Rosin–Rammler distribution)	n = 1.05771, b = 0.04282
Curing temperature	20 °C

Table 5. Mechanical Properties of the Cement Paste Constituents (see Z. Qian (2012))

No.	Element Type	Young Modulus E	Shear Modulus G	Tensile Strength *ft*	Compression Strength *fc*
		GPa	GPa	GPa	GPa
1	Unhydrated cement	135	52	1.8	-18
2	Interface Unhydrated and Inner	49	20	0.24	-24
3	Inner product	30	12	0.24	-24
4	Interface Inner and Outer	25	10	0.15	-1.5
5	Outer product	22	8.9	0.15	-1.5
6	Interface Outer and CH	26.4	10.6	0.15	-1.5
7	(CH) Calcium Hydroxides	33	13.2	0.264	-2.64
8	Interface Unhydrated and Outer	38	15.2	0.15	-1.5
9	Interface Inner and CH	31.5	12.6	0.24	-2.4

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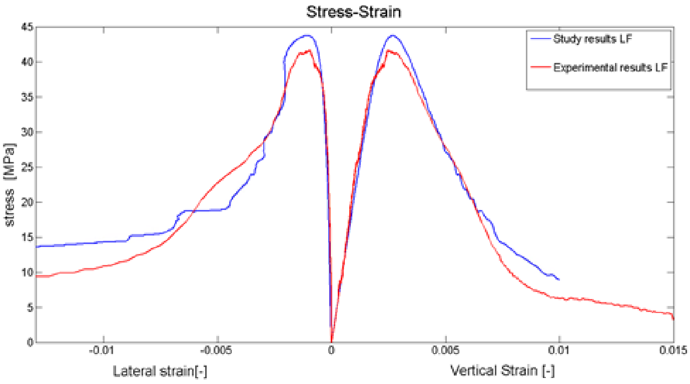

Figure 3. Uniaxial compression test; experimental and numerical results

The stress-strain curves that is presented in Figure 3, demonstrates that the discrepancy between the experimental results and the numerical results as excellent were 8 parameters were obtain from the lower scale properties. Therefore, we conclude that the proposed method of bridging the scales is an effective way to provide accurate results. More details can be found in Sherzer et al. (2017A, B)

DISCUSSION AND CONCLUSION

This paper presents a methodology for evaluating the nonlinear properties of concrete based on the cement paste chemical and mechanical properties.

The tensile and the shear parameters obtained from microscopic simulations of the cement paste, sand and mortar scales, while the compression parameters obtain from microscopic simulations of the cement paste scale. Further research is required to enable upscaling the full set of the LDPM parameters related to the friction and interaction phenomena.

This methodology provide the basis for a powerful design tool, which illuminate the influence of the lower scales on the concrete macroscopic strength.

ACKNOWLEDGMENTS

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References

1. Bažant, Z.P.; Pijaudier-Cabot, G. Measurement of characteristic length of nonlocal continuum. J. Eng. Mech. 1989, 115, 755–767
2. Cusatis, G.; Pelessone, D.; Mencarelli, A.: Lattice discrete particle model (LDPM) for failure behavior of concrete. I: Theory. Cement and Concrete Composites. 33 (9), 881-890 (2011).
3. Cusatis, G.; Mencarelli, A.; Pelessone, D.; Baylot, J.: Lattice Discrete Particle Model (LDPM) for failure behavior of concrete. II: Calibration and validation. Cement and Concrete composites. 33 (9), 891-905 (2011).
4. Garboczi, E. J.; Bentz, D. P.: Computer simulation and percolation theory applied to concrete. Annual Reviews of Computational Physics VII. 85 (1999).
5. Hofstetter, G.; and H. Mang, Computational mechanics of reinforced concrete structures: Vieweg+ Teubner Verlag, 1995.
6. Poinard, C.; Malecot, Y.; Daudeville, L.: Damage of concrete in a very high stress state: experimental investigation. Materials and Structures. 43 (1-2), 15-29 (2010).
7. Qian, Z.; Schlangen, E.; Ye, G.; Van Breugel, K.: Multiscale lattice fracture model for cement-based materials. IN: ICCM 2012: 4th International Conference on Computational Methods, Gold Coast, Australia, ICCM: Gold Coast, Australia, 2012; pp 25-28
8. Qian, Z.; Multiscale modeling of fracture processes in cementitious materials. Ph.D. Thesis, Delft University of Technology, Delft, The Netherlands, 2012.
9. Qian, Z.; Garboczi, E.; Ye, G.;Schlangen, E. Anm: A geometrical model for the composite structure of mortar and concrete using real-shape particles. Mater. Struct. 2016, 49, 149–158 (2016).
10. Sherzer, G.; Marianchik, E.; Cohen, R.; Gal, E.; Development, Calibration, and Validation of Lateral Displacement for a Concrete Uniaxial Compression Test. In CONCREEP 10, , Vienna University of Technology, Austria, 2015 pp 1420-1429.
11. Sherzer, G.; Gao, P.; Schlangen, E.; Ye, G.; Gal, E.; Upscaling Cement Paste Microstructure to Obtain the Fracture, Shear, and Elastic Concrete Mechanical LDPM Parameters. Materials. 10 (3), 242 (2017).
12. Sherzer, G.; Gao, P.; Schlangen, E.; Ye, G.; Gal, E.; Microstructure Upscaling to Obtain the Compressive Mechanical Parameter of the Lattice Discrete Particle Model. Presented at the The 4th MC meeting of the COST Action TU1404 in conjunction with the 2nd International RILEM/COST Conference on Early Age Cracking and Serviceability in Cement-based Materials and Structures, Brussels, Belgium 2017.
13. Vu, X. H.; Malecot, Y.; Daudeville, L.; Buzaud, E.: Effect of the water/cement ratio on concrete behavior under extreme loading. International Journal for Numerical and Analytical Methods in Geomechanics. 33 (17), 1867-1888 (2009).
14. Van Breugel, K.; Numerical simulation of hydration and microstructural development in hardening cement-based materials (I) theory. Cement and Concrete Research. 25 (2), 319-331 (1995).
15. Ye, G.; Van Breugel, K.; Fraaij, A.: Three-dimensional microstructure analysis of numerically simulated cementitious materials. Cement and Concrete Research. 33 (2), 215-222 (2003).