Assessing properties of hydrating cement paste using X-ray computed tomography characterization

Zhang, H.; Schlangen, E.; Ge, Zhi; Šavija, B.

Publication date
2021

Document Version
Final published version

Published in
4th International Rilem Conference on Microstructure Related Durability of Cementitious Composites

Citation (APA)
Zhang, H., Schlangen, E., Ge, Z., & Šavija, B. (2021). Assessing properties of hydrating cement paste using X-ray computed tomography characterization. In G. Ye, H. Dong, J. Liu, E. Schlangen, & C. Miao (Eds.), *4th International Rilem Conference on Microstructure Related Durability of Cementitious Composites: Microdurability 2020* (pp. 440-445). Delft University of Technology.

ASSESSING PROPERTIES OF HYDRATING CEMENT PASTE USING X-RAY COMPUTED TOMOGRAPHY CHARACTERISATION

H.Zhang (1,2), E. Schlangen (1), Z. Ge (2) and B. Šavija (1)

(1) Materials & Environment, Delft University of Technology, The Netherlands

(2) School of Qilu Transportation, Shandong University, China

Abstract

Properties of concrete are, to a large extent, dependent on the properties of its binding constituent, hydrated cement paste. Therefore, knowledge of properties of hydrated cement paste is crucial for predicting concrete behaviour. This paper presents an experimentally informed approach for modelling elastic and transport properties of cement paste. The models used realistic microstructural information-obtained by X-ray computed tomography-as input for property determination. The properties were then determined using discrete numerical models, namely, models based on a lattice approach. Modelling results were compared with literature data, showing excellent correlations. Furthermore, dependence of properties of cement paste on the total porosity, based on the modelling results, was explored. Finally, a correlation between elastic and transport properties for the explored range of Portland cement pastes was established. It is seen that the models can be used for property prediction, but also for exploring correlations between different parameters.

Keywords: Cement paste, Young's modulus, Chloride diffusion; Lattice model, X-ray computed tomography

1. INTRODUCTION

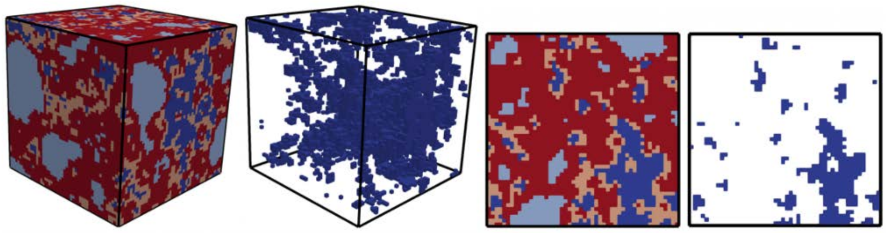
Understanding properties of concrete and their development in time is of great interest. Properties of concrete are, to a great extent, determined by the properties of its main constituent – cement paste [1]. This is valid for the mechanical properties, such as strength [2] and elastic modulus [3], but also for the durability, measured through e.g. transport properties such as permeability [4]. Simulation and prediction of property development in cement pastes is therefore a major topic of research in the field of cementitious materials.

In the past decade or so, numerous approaches for simulating property development of cement paste have been proposed. In general, these approaches comprise two parts: simulation of hydration and microstructure development, and simulation of the property (e.g. elastic modulus, strength, or diffusivity) itself.

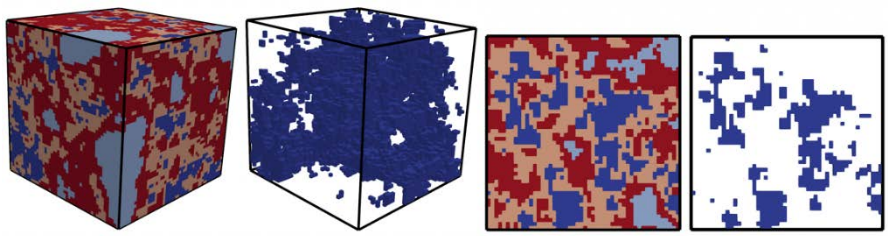
In this work, experimentally obtained microstructures are used as input for simulating transport (diffusivity) and mechanical (elastic modulus) properties of cement pastes of various ages. Simulation results are first validated by comparing them to experimental observations. Then, properties of cement pastes for different w/c ratios and ages are determined. This work has two aims: first, it tries to establish the experimentally-informed modelling procedure as a viable option for obtaining properties of multi-phase porous materials such as cement paste and second, it explores relationships between mechanical and transport properties (chloride diffusivity) of cement paste.

2. EXPERIMENTS

X-ray computed tomography was performed on micro-beam specimens with 500 µm × 500 µm cross section. Specimens were prepared for w/c ratio of 0.3, 0.4 and 0.5 and testing age of 7, 28 and 60 d. The specimen preparation procedure and scanning set-up are described in detail in [5]. The resulting digital material structure has a resolution of 2 µm/voxel. Image segmentation was then processed to segment the material structure into different phases: pore phase, the outer hydration product phase, the inner hydration product phase, and unhydrated cement phase. From each scanned image, 10 cubic subsamples of 100 × 100 × 100 µm3 (i.e. 50 × 50 × 50 voxels) were extracted to be used for numerical simulations. Examples of the microcubes are shown in Fig. 1 for 7 days of hydration, respectively. Properties of each micro-cube were simulated in 3 orthogonal directions, to capture the anisotropy in the material behavior. This provided 30 measures for the elastic modulus and chloride diffusivity for each w/c ratio and testing age.



(a) w/c=0.3



(b) w/c=0.4

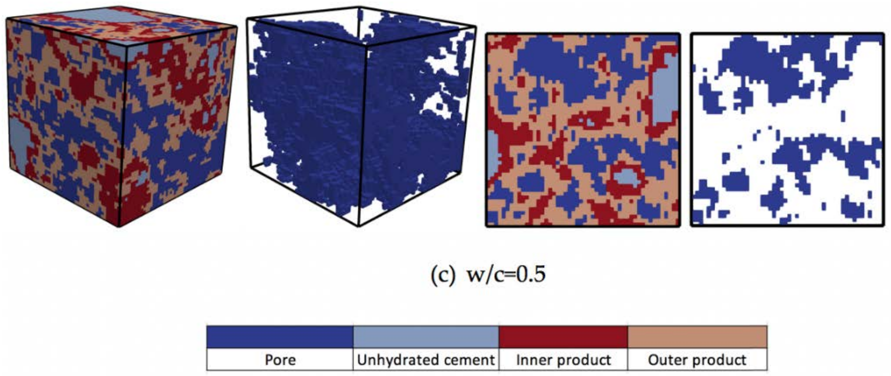


Figure 1: Examples of 100 × 100 × 100 µm^3 cement paste microcubes obtained from X-ray computed tomography after 7 days of hydration and subsequently segmented. Left to right: complete microstructure; only pores; 2D of the microstructure; 2D slice showing only the pores

3. MODELLING

In recent years, discrete models have been used to simulate transport processes in concrete [6-8]. Furthermore, coupled mechanical and transport models, which consider the effect of cracking on transport, have been developed [9-12]. In the mechanical lattice model, the continuum is discretized as a set of truss or beam elements that can transfer forces. On the other hand, in the transport lattice model, the continuum is discretized as a set of one dimensional conduit ("pipe") elements through which the transport takes place. In the current study, the approach described in [13] was used to calculate the Young's modulus and chloride diffusion coefficient of the microcubes.

4. RESULTS

In Fig. 2, simulated Young's moduli for all microcubes are plotted as a function of the total porosity. The Young's modulus of cement paste is approximately an exponential function of the porosity, i.e. of the following form:

$$E = ae^{bP} \tag{1}$$

Here, E is the Young's modulus of cement paste (GPa), a and b are the fitting parameters, and P the porosity (%). For the considered cement pastes, the fitting coefficients are a=38.76 and b=-0.04418 and the coefficient of determination is R^2=0.9337. Note that the linear fit is valid for all w/c ratios and ages: in other words, the Young's modulus of considered cement pastes is dominantly a function of porosity. Relative amounts of solids (i.e. unhydrated particles and hydration products) in the skeleton is of secondary importance for the Young's modulus of the composite according to the model since the Young's moduli of individual hydration phases are relatively similar, especially the inner and the outer product, while the amount of unhydrated cement is small. An exponential relation between porosity and Young's modulus has been proposed previously in the literature. For example, Spriggs [14] showed that the relation is valid for refractory materials. Note that this relation is purely empirical and, although it is valid for a practical range of porosities, it does not satisfy the physical condition that, for a 100% porosity, a zero elastic modulus should be obtained [15].

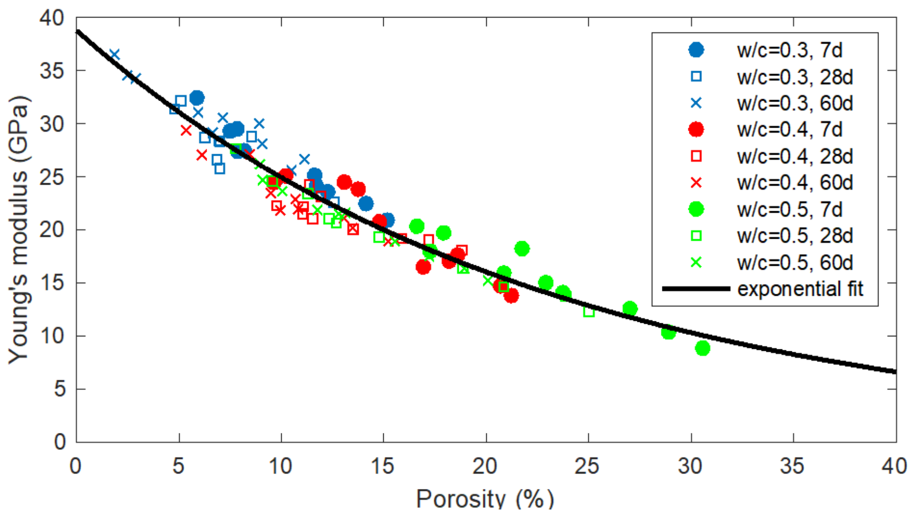


Figure 2: Young's modulus as a function of total porosity

In Fig. 3, chloride diffusion coefficient for all microcubes is plotted as a function of total porosity. It can be seen from Fig. 3 that the chloride diffusion coefficient of hydrated cement paste is dependent on the porosity in an approximately exponential way. An exponential relation between the porosity and the chloride diffusion coefficient is determined through regression analysis as follows:

$$D = ae^{bP} \quad (2)$$

where D is the diffusion coefficient (in 10^{-12} m^2/s), a and b fitting parameters, and P the porosity (%). For the considered cement pastes, a=1.192 and b=0.07852, with a coefficient of determination R^2=0.9164. The exponential fit is also shown in Fig. 3.

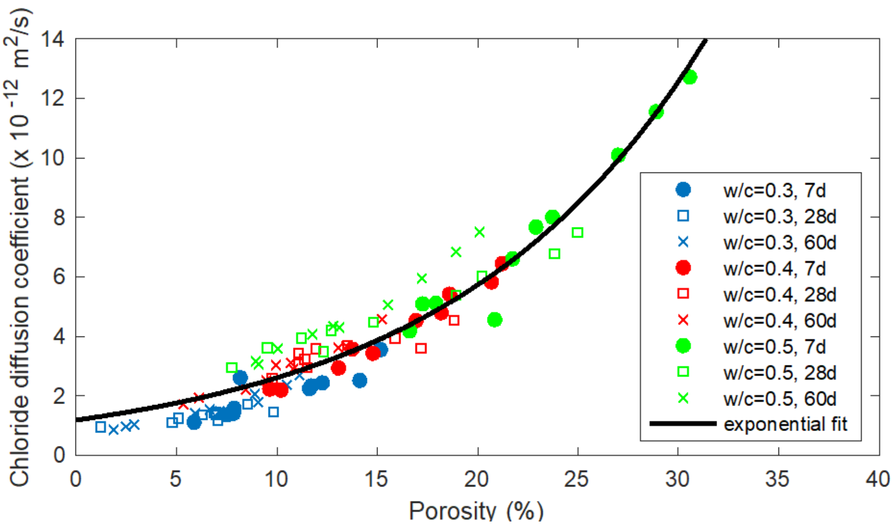


Figure 3: Chloride diffusion coefficient as a function of total porosity

It is clear that both the Young's modulus and the chloride diffusivity of hydrated Portland cement paste are dependent on the microstructure, especially the porosity. However, while Young's modulus decreases exponentially with increasing porosity (Fig. 2), the chloride diffusion coefficient shows an exponential increase with increasing porosity (Fig. 3). Therefore, for the ordinary Portland cement pastes considered, it may be possible to define a relationship between the Young's modulus and the chloride diffusion coefficient. In Fig. 4, a relationship between the calculated Young's modulus and calculated chloride diffusion coefficient for each microcube is plotted.

It can be seen that an approximately power relation exists between the two variables. This relation can be written as:

$$D = kE^m \quad (3)$$

where k and m are fitting parameters. For the microstructures considered, k=429.3 and m=-1.564, and the power fit has a coefficient of determination R^2=0.8534. The fitting relation is also shown in Fig. 4.

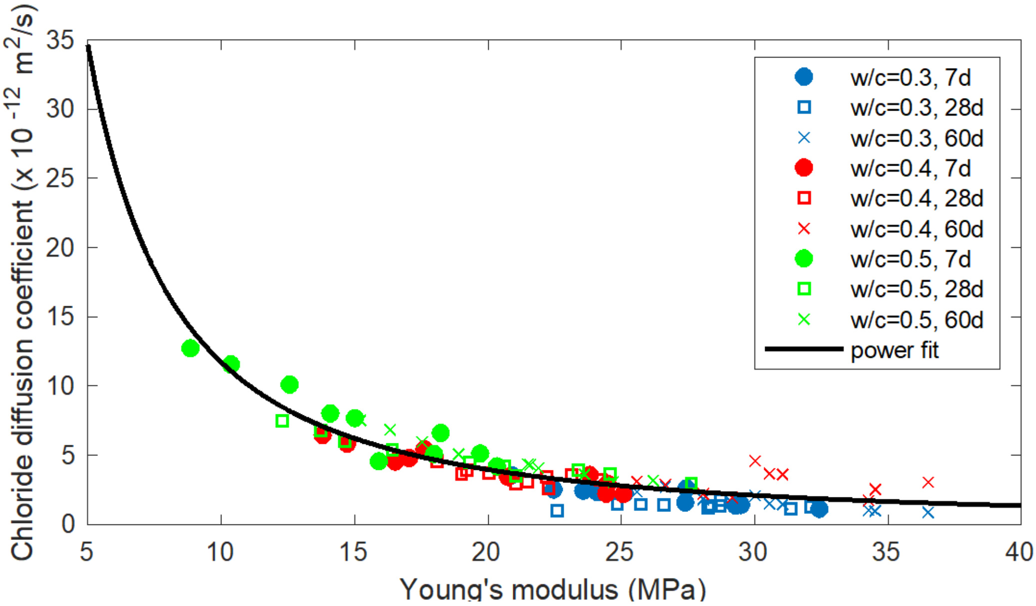


Figure 4: Relationship between the Young's modulus and the chloride diffusion coefficient for hydrated cement pastes considered.

5. CONCLUSIONS

In this work, an experimentally-informed modelling approach for determining elastic (Young's modulus) and transport (chloride diffusivity) properties has been proposed. The models use X-ray computed tomography data as microstructural input. Both the mechanical and the transport model use a discrete (lattice) approach to discretize the material domain and simulate different phases in the microstructure. Microstructure-property relationships and their time dependence were explored. Finally, a correlation between Young's modulus and chloride diffusivity in ordinary Portland cement pastes has been discussed.

ACKNOWLEDGEMENTS

This work has been financially supported by a European Union Horizon 2020 project InnovaConcrete (Innovative Materials and Techniques for the Conservation of 20th Century Concrete-Based Cultural Heritage), Grant Agreement Number 760858. H. Zhang would like to acknowledge the financial support of China Scholarship Counsil (CSC) under the grant CSC No.201506120067 and Taishan Scholars Program of Shandong province under the grant number tsqn201909032. Arjan Thijssen has performed the X-ray computed tomography experiments and his assistance is gratefully acknowledged.

REFERENCES

[1] T.C. Powers, T.L. Brownyard, Studies of the physical properties of hardened Portland cement paste, Journal Proceedings, 1946, pp. 101-132.

[2] H.A. Toutanji, T. El-Korchi, The influence of silica fume on the compressive strength of cement paste and mortar, Cement Concrete Res 25(7) (1995) 1591-1602.

[3] T.J. Hirsch, Modulus of elasticity of concrete affected by elastic moduli of cement paste matrix and aggregate, Journal Proceedings, 1962, pp. 427-452.

[4] G. Ye, Experimental study and numerical simulation of the development of the microstructure and permeability of cementitious materials, TU Delft, Delft University of Technology, 2003.

[5] H. Zhang, B. Šavija, S.C. Figueiredo, E. Schlangen, Experimentally validated multi-scale modelling scheme of deformation and fracture of cement paste, Cement Concrete Res 102 (2017) 175-186.

[6] S.D. Abyaneh, H. Wong, N. Buenfeld, Computational investigation of capillary absorption in concrete using a three-dimensional mesoscale approach, Comp Mater Sci 87 (2014) 54-64.

[7] B. Šavija, M. Luković, E. Schlangen, Lattice modeling of rapid chloride migration in concrete, Cement Concrete Res 61 (2014) 49-63.

[8] L. Wang, T. Ueda, Mesoscale modeling of water penetration into concrete by capillary absorption, Ocean Eng 38(4) (2011) 519-528.

[9] D. Asahina, J.E. Houseworth, J.T. Birkholzer, J. Rutqvist, J. Bolander, Hydro-mechanical model for wetting/drying and fracture development in geomaterials, Comput Geosci 65 (2014) 13-23.

[10] P. Grassl, J. Bolander, Three-dimensional network model for coupling of fracture and mass transport in quasi-brittle geomaterials, Materials 9(9) (2016) 782.

[11] M. Luković, B. Šavija, E. Schlangen, G. Ye, K. van Breugel, A 3D lattice modelling study of drying shrinkage damage in concrete repair systems, Materials 9(7) (2016) 575.

[12] N. Benkemoun, M.N. Hammood, O. Amiri, A meso-macro numerical approach for crack-induced diffusivity evolution in concrete, Constr Build Mater 141 (2017) 72-85.

[13] B. Šavija, H. Zhang, E. Schlangen, Assessing Hydrated Cement Paste Properties Using Experimentally Informed Discrete Models, J. Mater. Civ. Eng. 31(9) (2019) 04019169.

[14] R. Spriggs, Expression for effect of porosity on elastic modulus of polycrystalline refractory materials, particularly aluminum oxide, J Am Ceram Soc 44(12) (1961) 628-629.

[15] D. Hasselman, On the porosity dependence of the elastic moduli of polycrystalline refractory materials, J Am Ceram Soc 45(9) (1962) 452-453.