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# MICROSTRUCTURE-BASED MODELLING OF TRANSPORT PROPERTIES IN NON-SATURATED CEMENTITIOUS MATERIALS

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ABSTRACT: Transport properties (e.g. permeability and diffusivity) of cementitious materials are usually considered as the main indicators for durability assessment and service life prediction of reinforced concrete structures. In practice, concrete is rarely saturated. Therefore, it is not only of scientific interest but of practical importance to study transport properties in non-saturated cementitious materials. In principle, an ideal model for transport properties should account for the 3D microstructure, especially the pore structure of cementitious materials. This study presents an integrated modelling scheme to estimate the transport properties of cementitious materials with various saturation levels based on their microstructures. The 3D microstructure of cement paste is obtained from high-resolution X-ray computed microtomography. An in-house code based on single-phase and multiphase lattice Boltzmann models is developed and used to simulate the moisture distribution, water permeability and ionic diffusivity of cement paste with different curing ages. Afterwards, the effects of moisture content and microstructure of cement paste on its permeability and ionic diffusivity are investigated in a quantitative manner. The results indicate that the moisture distribution, permeability and ionic diffusivity of non-saturated cement paste significantly depend on its 3D microstructure, in particular effective porosity. A unique relationship between transport properties and effective porosity can be found. The simulated results show a good agreement with experimental data. The proposed modelling scheme provides an effective tool to predict the transport properties in non-saturated cementitious materials.
Keywords: Cement paste, microstructure, permeability, diffusivity, X-ray computed tomography.

## INTRODUCTION

Concrete is used in the construction of a wide range of structures. During service, concrete may interact with its environment. For instance, the aggressive chemical species (e.g. chloride, sulfates, carbon dioxide, etc.) from the environment can penetrate into the concrete, thereby leading to a series of degradation processes of the concrete itself or the reinforcement embedded in the structures. These degradation processes strongly relate to the transport phenomena in concrete and transport properties of concrete, e.g. permeability and diffusivity, are usually considered as indicators to evaluate the durability and predict the service life of reinforced concrete structures. In practice, concrete is rarely in a state of full saturation during construction and throughout its long lifetimes due to self-desiccation and wetting-drying cycles. In addition, the corrosion of reinforcing steel in concrete occurs only in an unsaturated state, whereby the oxygen can get access to the rebar surface. Therefore, it is vital to estimate transport properties of partially saturated cementitious materials in order to make an accurate prediction of service life and assessment of durability of reinforced concrete structures.

In recent years, an increasing attention has been paid to transport properties in non-saturated cementitious materials. Although many efforts including experimental and modelling work have been conducted to qualitatively or quantitatively investigate the effect of moisture content on transport properties (See [1] for a critical review of these existing efforts), to what extent does the water saturation influence transport properties in still unclear as results published so far show a great dispersion. This can be ascribed to the complexity of microstructure of cementitious materials. The main purpose of this study is to quantitatively investigate the effect of degree of water saturation on transport properties in cementitious materials taking into account the 3D microstructure.

## 3D MICROSTRUCTURE OF CEMENT PASTE

In this study, the 3D microstructure of cement paste was obtained from X-ray computed microtomography (XCT) scans. ASTM type I Portland cement was used. The w/c ratio of the cement paste was 0.5 (mass ratio). After drill mixing in a plastic beaker, small parts of the paste were poured into the syringe and then injected into a micro plastic tube with an internal diameter of 250 µm. The specimen was stored in the standard curing room with a relative humidity of 95% and temperature of 20 ºC and scanned at 1, 7 and 28 days. More details about the XCT testing can be found in [2]. Fig.1 shows the XCT grey image of a cylindrical region of interest (ROI) of 28-day old cement paste with 200 µm in diameter and 100 µm in thickness extracted from the centre of the reconstructed 3D images where the cement paste is considered to be most homogeneous. The phases in dark, white and grey represent capillary pore, anhydrous cement grains and hydration products, respectively. In order to identify these three phases in cement phase and quantify the microstructural information, a series of image processing and analysis are required, the details of which were given in [3]. The segmented capillary pore of 28-day old cement paste corresponding to the original image in Fig.1 is shown in Fig. 2. For following simulations, a cubic volume of interest (VOI) of 100 × 100 × 100 µm$^3$ is extracted from the centre of ROI, as shown in Fig. 3.

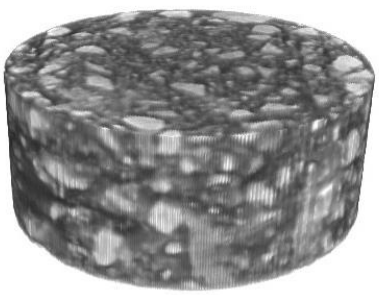

**Fig. 1:** *XCT image of 28-day old cement paste*

**Fig. 2:** *Pore structure of ROI of 28-day old cement paste*

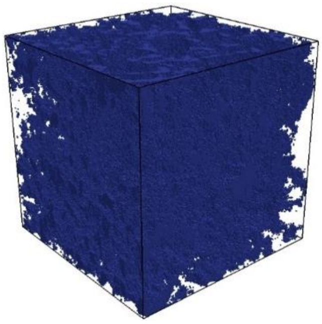

**Fig. 3:** *Pore structure of VOI of 28-day old cement paste*

## MICROSTRUCTURE-BASED MODELLING

The entire modelling procedure for transport properties in unsaturated cement paste consists of the following four main steps:

(1) Mapping of 3D microstructure onto a discrete cubic lattice with a 1-to-1 correlation of voxel-to-node [4]. The pore voxels are considered as fluid nodes. The solid voxels composed of hydration products and anhydrous cement grains are regarded as impermeable solid nodes.

(2) Modelling equilibrium distribution of moisture in cement paste with various degrees of water saturation using multiphase lattice Boltzmann method (LBM). The fluid nodes in the cubic lattice are initially saturated with a random homogeneous mixture of water and gas phases with a specific

volume ratio corresponding to a given degree of water saturation, $S_w$. An example of the initial random distribution of moisture at $S_w$ = 75% in pore structure is shown in Fig. 4. Liquid water and gas are represented in blue and white, respectively. Afterwards, the interactions between water/gas and solid are simulated using multiphase LBM. The reader is referred to [5] for more details.

(3) Modelling water permeation through cement paste at various moisture levels using single-phase multi-relaxation-time LBM (see [6] for further information) and calculating the corresponding water permeability as a function of degree of water saturation.

(4) Modelling ionic diffusivity using LBM for diffusion, the details of which can be found in [7].

## RESULTS AND DISCUSSION

Fig. 5 shows the equilibrium distribution of moisture in pore network of 28-day old cement paste with water saturation of 75% corresponding to the initial random distribution of moisture in Fig. 4. The liquid water covers the solid surface and tends to fill the pores with smaller size, while the gas phase tends to occupy the central region of larger pores and forms many gas phase clusters. The water-filled pores provide possible paths for water movement and ion transport, as shown in Fig.6.

With the obtained equilibrium distribution of moisture in cement paste at various saturation levels, the water permeation and ionic diffusion through unsaturated cement paste can be subsequently simulated following the Steps (3) and (4). Figs. 7 and 8 respectively show the steady-state streamline along the flow direction and ionic diffusion concentration along the diffusion direction from left to right within 28-day old cement paste at water saturation of 75%.

Figs. 9 and 10 show the relative water permeability and ionic diffusivity of cement paste with various curing ages and w/c ratios against water saturation. When the water saturation decreases from 100% to around 70%, transport properties drop sharply, followed by a less obvious decrease until the critical water saturation. Transport properties at various saturation states highly depend on the 3D microstructure. The simulation results agree very well with experimental data.

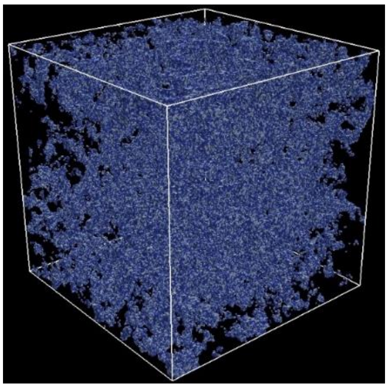

**Fig. 4:** *Initial random distribution of water and gas in pore structure*

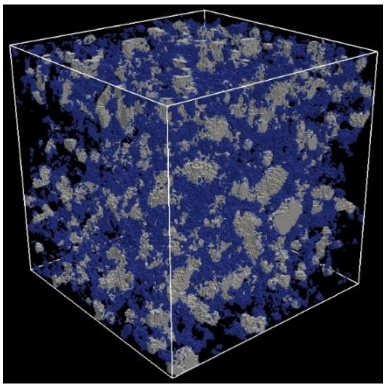

**Fig. 5:** *Equilibrium distribution of water and gas in pore structure*

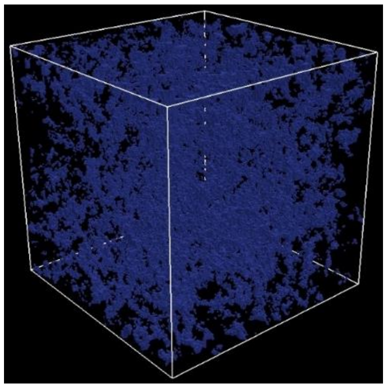

**Fig. 6:** *Liquid water-filled pores in pore structure*

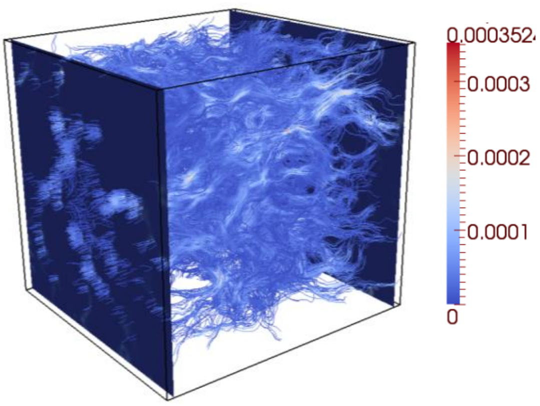


**Fig. 7:** *Steady-state flow through pore structure*

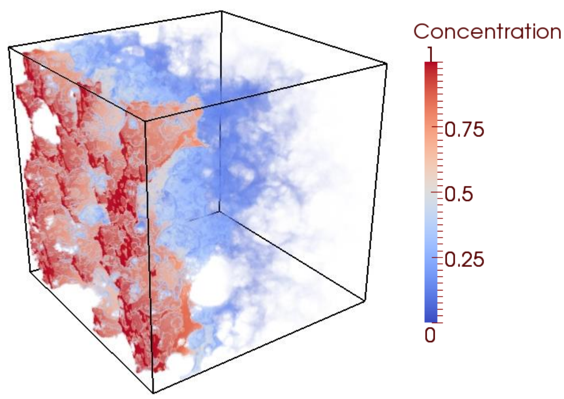


**Fig. 8:** *Ionic concentration distribution in pore structure*

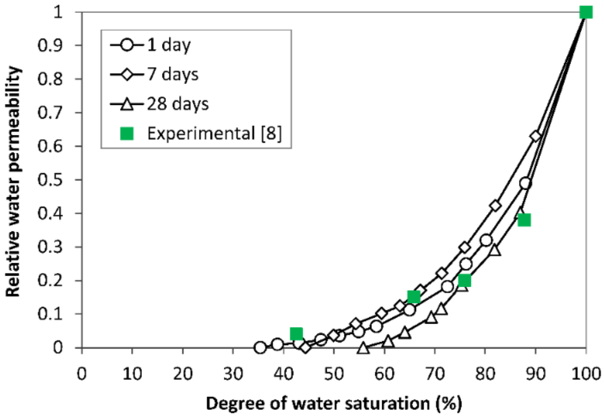

**Fig. 9:** *Relative permeability against saturation levels*

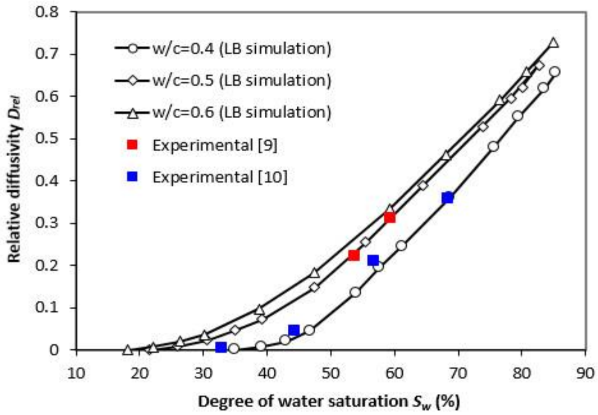

**Fig. 10:** *Relative ionic diffusivity again saturation levels*

## CONCLUSIONS

In this study, an integrated modelling approach is presented to investigate transport properties of partially saturated cementitious materials in a quantitative manner. The equilibrium 3D distribution of moisture in cement paste at various saturation levels can be successfully obtained. Transport properties strongly depend on both degree of water saturation and 3D microstructure.

## REFERENCES

[1] Zhang Y and Zhang M. Transport properties in unsaturated cement-based materials – A review. *Construction and Building Materials*, 2014, 72 367-379.

[2] Zhang M, He Y, Ye G, Lange D A and van Breugel K. Computational investigation on mass diffusivity in Portland cement paste based on X-ray computed microtomography (CT) image. *Construction and Building Materials*, 2012, 27 472-481.

[3] Zhang M and Jivkov A P. Micromechanical modelling of deformation and fracture of hydrating cement paste using X-ray computed tomography characterisation. *Composites Part B: Engineering*, 2016, 88 64-72.

[4] Zhang M. *Multiscale lattice Boltzmann-finite element modelling of transport properties in cement-base materials*, PhD Thesis. Delft University of Technology, The Netherlands 2013.

[5] Zhang M, Xu K, He Y and Jivkov A P. Pore-scale modelling of 3D moisture distribution and critical saturation in cementitious materials. *Construction and Building Materials*, 2014, 66 222-230.

[6] Zhang M, Ye G and van Breugel K. Microstructure-based modeling of permeability of cementitious materials using multiple-relaxation-time lattice Boltzmann method. *Computational Materials Science*, 2013, 68 142-151.

[7] Zhang M, Ye G and van Breugel K. Modeling of ionic diffusivity in non-saturated cement-based materials using lattice Boltzmann method. *Cement and Concrete Research*, 2012, 42 1524-1533.

[8] Kameche Z A, Ghomari F, Choinska M and Khelidj A. Assessment of liquid water and gas permeabilities of partially saturated ordinary concrete. *Construction and Building Materials*, 2014, 65 551-565.

[9] Nielsen E P and Geiker M R. Chloride diffusion in partially saturated cementitious materials. *Cement and Concrete Research*, 2003, 33 133-138.

[10] de Vera G, Climent M A, Viqueira E, Anton C and Andrade C. A test method for measuring chloride diffusion coefficients through non-saturated concrete. Part II: The instantaneous plane source diffusion case with chloride binding consideration. *Cement and Concrete Research*, 2007, 37 1113-1123.