

Two-scale modeling of transport properties of cement paste: Formation factor, electrical conductivity and chloride diffusivity



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ABSTRACT

Predicting transport properties of cement-based materials directly from the microstructure is very challenging, due to the problems of bridging length scales and the difficulties of realistically representing the microstructure. Based on a two-scale representation of the microstructure, a scheme is proposed in this paper to model the transport properties of cement paste through two-scale random walk simulation. A random walk algorithm is firstly applied at the sub-micro-scale to determine the diffusion tortuosity of the outer C-S-H layer. This is then up-scaled to the micro-scale to compute the diffusion tortuosity of cement paste. Based on physical laws, the diffusion tortuosity is transformed into the formation factor, and further into the electrical conductivity and the chloride diffusion coefficient of cement paste, and subsequently validated. It is proven that a more realistic representation of the microstructure makes it possible to derive transport properties of cement paste, directly and accurately, from the microstructure.

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1. Introduction

The increased emphasis on the sustainable development of building projects requires that more and more attention is paid to the service life and durability of concrete structures. It has been well recognized that durability is most influenced by the transport properties of concrete [1]. “Transport properties of concrete” is a broad term that covers all properties involving the transport of fluids or ions in concrete. The fluids which are relevant to durability include, but are not limited to, water (pure or containing aggressive ions), carbon dioxide and oxygen [2]. They can move into and through concrete in different ways, but almost all transport properties depend primarily on the pore structure of concrete.

Many researchers have tried to predict transport properties based on measured pore structure parameters and assumed, reconstructed or simulated microstructures, through empirical, analytical or numerical methods. Empirical models include linear relations between conductivity/diffusivity and pore structure parameters [3–5], power law relations between permeability and pore structure parameters [2,6], as well as some multi-parameter models [7–9]. These models are difficult to be generally valid, as they are developed from average or equivalent parameters, rather

than from the actual microstructure. On assumed [10–13] or reconstructed pore structures [14–16], physical laws are frequently applied to solve the transport properties of cement-based materials. Numerical methods, including finite element methods, finite difference methods and the random walk algorithm, have also been employed to compute transport properties based on the microstructures simulated by computer models or obtained through experiments [17–22]. The most promising methods for predicting transport properties seem to be ones deducing properties directly from realistically represented microstructures [23].

Although the microstructure of cement-based materials has been well described in the light of experiments as well as computer models [24–30], and some promising studies have been done [31], predicting transport properties directly from the microstructure is still a big challenge for the future, especially at the cement paste level [23]. This is mainly due to the problems of bridging length scales in such a material whose microstructure is manifested at several length scales [32–36]. Even though the capillary pores in cement paste is simply considered, their sizes cover the range from less than 10 nm to larger than 10 μm , spanning 4–5 orders of magnitude [37]. The representative elementary volume (REV) for cement paste is generally regarded to be 100–300 μm [23,26,29], while the smallest important features are normally below 0.1 μm in size [23]. Thus when simulating the microstructure of cement paste for the purpose of computing transport

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properties, the representability and resolution are difficult to be guaranteed at the same time, to say nothing of accurately deducing properties from the microstructure.

Recently, a computer model has been developed to simulate the capillary pores in hydrated cement paste at two scales, i.e. small capillary pores (SCPs) at the sub-micro-scale covering features from 10^{-9} m to 10^{-6} m, and large capillary pores (LCPs) at the micro-scale covering features from 10^{-7} m to 10^{-4} m [38]. In this way, representability and resolution can be guaranteed at each scale, so that the capillary pore structure can be represented more realistically. The present study aims to deduce the transport properties of cement paste based on the microstructure simulated by the two-scale model. From the simulated microstructures, random walk simulation is employed to determine the diffusion tortuosity at the sub-micro-scale, which is later up-scaled to the micro-scale to compute the diffusion tortuosity of cement paste. The diffusion tortuosity is further transformed to the formation factor of cement paste, from which the electrical conductivity and steady state chloride diffusion coefficient can be calculated. The formation factor can certainly be transformed to other transport properties, i.e. the intrinsic permeability [39,40], but that is out of scope of the present paper. Finally, the model is validated by comparing the computed results with experimentally measured electrical conductivities and chloride diffusion coefficients.

2. Materials and experiments

To validate the proposed model, cement pastes were prepared, and their electrical conductivities were measured following increasing ages. Cement satisfying the requirements of BS EN197-1:2000 for CEM I Portland cement of strength class 52.5 N was used in this study, and the considered water-to-cement ratios included 0.3, 0.4 and 0.5. The chemical composition of the cement is listed in Table 1. Cement pastes, with different water-to-cement ratios, were mixed, cast into steel molds of dimensions of 40 mm × 40 mm × 160 mm, and sealed by plastic sheet to prevent water evaporation from the specimens. After 24 h, the specimens were de-molded and immersed in saturated calcium hydroxide solution at 25 ± 2 °C. At the ages of 1, 3, 7, 28, 60 and 120 days, the paste specimens were taken out, and measured for direct current electrical conductivity, as shown Fig. 1. After being surface-dried by a towel, a specimen was clamped between two spring-loaded stainless steel electrodes. Two pieces of thin sponge saturated with calcium hydroxide solution were inserted between each electrode and the specimen. The electrodes were then connected to an impedance analyzer for impedance spectroscopy measurement, according to the method used by Shane et al. [41]. The direct current electrical resistance of each sample was taken at the real impedance “cusp” between the bulk and electrode arcs on a Nyquist plot [42], and transformed to electrical conductivity. Three specimens were tested for each paste at a certain age, and the average values were determined and reported in this study.

3. Microstructure model

3.1. Basic assumptions

Previously, we proposed a two-scale model to simulate the microstructure of hydrated cement paste [38]. The nature of this

Table 1
Chemical composition of the cement (%).

CaO	SiO ₂	Al ₂ O ₃	Fe ₂ O ₃	SO ₃	MgO	Equivalent Na ₂ O	Free CaO	LOI
64.05	20.37	5.37	3.18	2.09	2.35	0.52	1	1.12

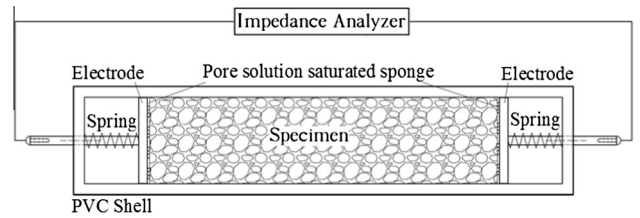


Fig. 1. Sketch of the setup for electrical conductivity measurement.

model was to arrange the capillary network in cement paste in a more realistic manner, by classifying capillary pores into small capillary pores (SCPs, from several to 100 nm) and large capillary pores (LCPs, >100 nm). SCPs are the capillary spaces in the outer hydration products layer formed due to the inadequate packing of hydration products, and LCPs are the spaces originally occupied by water but still not reached by hydration products, as shown in Fig. 2. It was also assumed that the capillary pores do not exist in the inner hydration products layer, or inside the original boundary of the cement grains. According to the said formation mechanisms, there should not be a strict boundary between the SCPs and LCPs, and the afore-mentioned boundary of 100 nm was proposed based on a comprehensive discussion [37,38].

At the micro-scale, it is considered that cement paste consists of five phases, i.e. unhydrated cement cores, inner hydration products layers, outer C-S-H layers, micro-sized crystal hydrates and LCPs [38], as shown in Fig. 2. In the five phases, the outer C-S-H layer is a mixture of LD (low density) C-S-H and SCPs, and the micro-sized crystal hydrates include micro-sized calcium hydroxide, ettringite, etc. Both of the two phases are outer hydration products, just separating the micro-sized crystal particles makes it easy to model the left part at the sub-micro-scale. The inner hydration products layers are assumed to consist of HD (high density) C-S-H and nano-sized crystal hydrates, based on Chen et al.’s research [43]. In the aforementioned five phases, the unhydrated cement cores and micro-sized crystal hydrates particles are impenetrable. As compared with the large capillary pores and outer C-S-H layers, it can be assumed that the inner hydration products layers are also impenetrable, as they are mixtures of barely penetrable HD C-S-H and impenetrable crystal hydrates [37]. In this way, the transport pathway in a hydrated cement paste is governed by the large

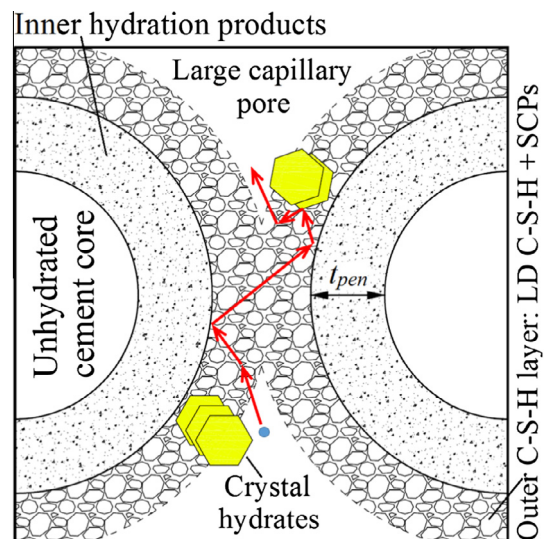


Fig. 2. Sketch of the microstructure and dominant transport pathway of cement paste at the micro-scale.

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