



Computational investigation of capillary absorption in concrete using a three-dimensional mesoscale approach



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ABSTRACT

In many exposure environments, capillary absorption of water controls the rate of deterioration of concrete. This paper presents a three-dimensional numerical investigation of capillary absorption by treating concrete as a heterogeneous composite discretised into a cubic lattice. The lattice elements were considered as conductive “pipes” with transport properties assigned based on the phase they represent. The capillary absorption process was described by a non-linear diffusion equation, with the hydraulic diffusivity a non-linear function of the degree of saturation of the composite. A non-linear finite element method was used to solve the governing differential equations. The numerical results were validated against analytical approximations, as well as experimental data from the literature. A sensitivity analysis was then performed to evaluate the effect of heterogeneities produced by aggregate particles on the absorbed water profile and the sorptivity coefficient. It was found that water penetrates concrete in an uneven profile influenced by the amount, spatial distribution and shape of the aggregate particles. Sorptivity decreased when spherical aggregate particles were replaced with ellipsoidal particles due to the consequent increase in tortuosity of the cement paste. This effect increased with increase in aspect ratio and volume fraction of aggregate. However, the size of aggregate particle appears to have an insignificant influence.

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1. Introduction

Most deterioration processes that affect concrete structures (e.g. reinforcement corrosion, sulphate attack, frost damage and leaching) occur as a result of intrusion of water. Water may be the main agent causing distress or may act as the transporting medium for aggressive species such as chlorides and sulphates. Therefore, the durability of concrete structures depends largely on its ability to resist the transport of water and dissolved aggressive species. Permeation, diffusion and absorption are three main transport mechanisms in cementitious materials. Permeation is the flow of fluids through a material under a pressure gradient, while diffusion is the movement of substances due to a concentration gradient. Absorption can be considered as the process of water uptake in a partially saturated material by means of capillary suction.

Many concrete structures in service experience wetting and drying cycles and so are rarely fully saturated. For example, basements and foundations experience fluctuating groundwater, and parts of marine and coastal structures are subjected to the tidal zone or salt

spray. In these environments, the ingress and accumulation of aggressive species are driven by the non-linear, capillary absorption process rather than a Fickian diffusion or pressure-induced flow. This nonlinearity comes from the dependence of moisture diffusivity on water content [1]. Obviously, a good understanding of moisture transport is important in order to assess performance, predict degradation and develop service life models and durability-based design codes. The performance of certain structures is dependent on the ability of concrete to remain watertight or provide a physical barrier to contaminants. Thus, it is highly desirable to be able to predict the depth of moisture penetration and solute concentration profile over time for a given concrete, condition and exposure environment.

Previous studies have been made to enhance our understanding concerning capillary absorption in cement-based materials. The approaches used can be categorised into experimental, analytical and numerical. Lab based transport testing has been performed for many years to gain a better understanding of different variables affecting capillary transport in cement-based materials [1–7]. Some researchers have proposed analytical approaches to model capillary absorption of water in porous materials. Hall et al. [8] analysed the absorption of water into porous material containing non-sorptive inclusions in terms of unsaturated flow theory and

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showed that sorptivity is reduced by a factor $1 - 1.25\alpha + 0.26\alpha^2$, where α is the volume fraction of inclusions. Although this equation was developed for the dilute case, it was found to be in good agreement with experimental data for gypsum plaster containing 2–49% sand volume fraction. In another study, Lockington et al. [9] proposed an analytical solution to predict water penetration profiles for unidirectional absorption in a homogeneous media. In this approach, hydraulic diffusivity is modelled by a nonlinear function of the degree of saturation. The predicted water penetration profiles were shown to be accurate by comparison against two sets of published experimental data for mortars.

The tremendous increase in computational capabilities has strongly favoured the development of numerical simulations based on a more precise description of microstructure. Numerical simulations should be able to give a more accurate prediction of effective properties of multiphase materials with complex internal microstructures compared to analytical predictions [10–12]. However, despite the numerous numerical modelling studies focusing on diffusion in cement-based materials, capillary absorption has received little attention [13–20]. Sadouki and van Mier [21] presented a flow model for simulating heat and mass transfer in heterogeneous materials. The material was discretised as a two-dimensional regular triangular lattice where the lattice elements are considered as conductive pipes. The model was then used to study the influence of the interfacial transition zone and non-saturated porous aggregate on moisture flow in concrete. More recently, Wang and Ueda [22] proposed a two-dimensional lattice network model to predict water penetration into concrete. Concrete was idealised at the mesoscale as a three-phase composite consisting of coarse aggregate, mortar and ITZ. The distribution of absorbed water content was calculated from the sorptivity and porosity of the mortar and ITZ phases.

There are significant advantages (and challenges) in simulating the capillary absorption process in three-dimensions, but to the best of our knowledge, this has not been reported before. Therefore, the aim of this work is to develop a framework to calculate the distribution of absorbed water content at any elapsed time given initial boundary conditions. The model will focus at the mesoscale, whereby concrete is idealised as a porous media containing aggregate particles of a range of size, shape and volume fraction, discretised into a lattice network. Water uptake by capillary absorption is described by a non-linear diffusion equation based on unsaturated flow theory, which is solved using a finite element method. A parametric study is then performed to evaluate the effect of heterogeneities produced by aggregate particles on the absorbed water profile and the sorptivity coefficient.

2. Unsaturated flow

This section provides a brief summary of the governing equations in the theory of unsaturated flow. For a more comprehensive treatment of the topic, readers are referred to previous reviews, for example by Hall [1,23]. Single-phase flow via capillary absorption in an unsaturated porous media is described by the extended Darcy equation:

$$\mathbf{q} = -K(\theta)\nabla\Psi(\theta) \quad (1)$$

where \mathbf{q} is the vector flow velocity, K is the hydraulic conductivity (L/T) and Ψ is the capillary potential (L). θ is the reduced water content defined as:

$$\theta = \frac{\Theta - \Theta_i}{\Theta_s - \Theta_i} \quad (2)$$

where Θ is the volumetric water content (i.e. ratio of volume of water to bulk volume of sample). Θ_i and Θ_s are the initial and

saturated volumetric water contents, respectively. Thus, θ equals zero initially and one at saturation.

It is often more convenient to express capillary absorption (Eq. (1)) in the form of a non-linear diffusion equation. This is obtained by combining Eq. (1) with the continuity equation and then rewriting the resultant equation in terms of θ by using the substitution $D(\theta) = K(\theta)(d\Psi/d\theta)$ giving the equation:

$$\frac{\partial\theta}{\partial t} = \nabla \cdot [D(\theta)\nabla\theta] \quad (3)$$

The hydraulic diffusivity D (L²/T) is a moisture and temperature dependent parameter, and is considered as the fundamental material property that describes the process of capillary absorption. Applying the Boltzmann transformation to Eq. (3) and integrating the resulting equation gives the following expression for $D(\theta)$:

$$D(\theta) = -\frac{1}{2} \frac{1}{(d\theta/d\phi)_0} \int_0^\theta \phi d\theta \quad (4)$$

Here, ϕ is the Boltzmann variable ($=x/t^{1/2}$) where x is the depth of water penetration and t is the elapsed time. $D(\theta)$ can be estimated by measuring water content versus distance profiles after various elapsed times using non-destructive test methods such as NMR or γ -ray attenuation. However, obtaining accurate water penetration profiles in cement-based materials is difficult and this is not commonly carried out. A simpler approach to determine $D(\theta)$ is through an approximation using an exponential function of θ :

$$D(\theta) = D_0 e^{n\theta} \quad (5)$$

in which D_0 is the limiting magnitude term and n is the shape term [24]. This exponential law has been shown to be valid for a range of construction materials including soils, brick, stone, gypsum and concrete. It has also been found that n varies little between materials, typically ranging from 6 to 8 [1,24–27]. Lockington et al. [9] showed that D_0 can be obtained from the conventional sorptivity test using the following equation:

$$D_0 = \frac{S^2}{(\Theta_s - \Theta_i)^2 (e^{n(2n^{-1} - n^{-2})} - n^{-1} + n^{-2})} \quad (6)$$

In the sorptivity test, a cylindrical sample is initially dried to a uniform moisture state and then a flat surface is exposed to free water (Fig. 1). The curved side surface is typically sealed with a waterproof coating (tape or epoxy) so that the uptake of water is approximately unidirectional in this arrangement. Gravitational effects are insignificant since water absorption in cement-based materials is dominated by capillary forces, at least for the short penetration distances during which sorptivity is measured. When these conditions are met, the cumulative mass of water absorbed per cross-section area I scales to $t^{1/2}$ and the sorptivity S can be determined from the slope of the best-fit line of:

$$I = St^{1/2} + A \quad (7)$$

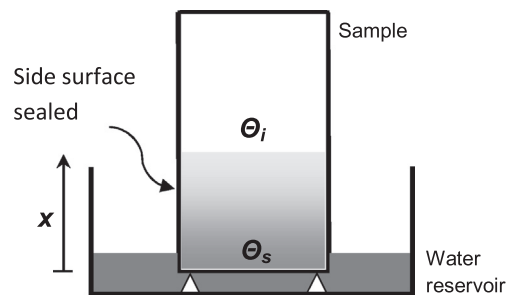


Fig. 1. Schematic of the sorptivity test.

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