- Technical Paper -

A TWO-PHASE ABSORPTION MODEL AND SIMULATION ON THE WATER ABSORPTION OF CRACKED ECC

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ABSTRACT

To simulate water absorption of cementitious materials with cracks, a two-phase model which treats cement matrix and cracks separately is proposed. Cracks are assumed smeared, and water transport is described by capillary suction pressure and saturation degree gradient. Water transport in cement matrix is simulated by an existing multi-scale model. Besides, cracks are regarded as reservoirs and to supply water to cement matrix continuously. Finally, the proposed model is verified by test of cracked Engineered Cementitious Composites (ECC), and the absorption process can be well simulated. Keywords: Water absorption, crack, ECC, capillary suction, multi-scale modeling

1. INTRODUCTION

Nowadays the durability of concrete structures is becoming an urgent and significant issue, with regard to the sustainability and ecology of human society. In contrast to cement matrix, cracks which occur due to external and environment loads are more vulnerable and accessible to water and harmful agents, causing the accelerated deterioration. Hence, in order to thoroughly evaluate the durability of structures, it is unavoidable and of great necessity to study water transport inside crack, as well as their influence on the cement matrix.

With the purpose of evaluating life-span performance of concrete materials and structures, a multi-scale computational system called DuCOM has been developed in Concrete Laboratory, the University of Tokyo [1]. Hydration, pore-structure formation, as well as water equilibrium and transport in cement matrix are coupled and simulated synthetically to attain water status in micropores. Furthermore, harmful substance ingression and accompanying deteriorations, such as carbonation, chloride penetration and steel corrosion, and calcium leaching are simulated. Verifications by tests show that this system provides proper simulations of deterioration phenomena in cement matrix and concrete.

In this paper, the authors focus on water absorption behaviors of cementitious materials with existence of cracks. In the occasion of immersion, because crack is much larger than micro-pores in dimension, capillary suction becomes drastic. Water can be absorbed and fill in cracks in quite short time, resulting in much accelerated absorption process. However, this capillary suction effect by cracks is not considered in the existing model, so the accelerated absorption cannot be simulated. Therefore, the authors attempt to establish a two-phase absorption model treating cement matrix and crack separately. The absorption by cement matrix still follows the existing model, and first of all it is briefly introduced.

2. WATER EQUILIBRIUM AND TRANSPORT MODEL IN CEMENT MATRIX [1, pp.121-161]

In DuCOM, micro-pores inside cement matrix are categorized as capillary, gel and interlayer pores. Their porosities are calculated according to hydration degree and intrinsic properties of gel grains. Interlayer pores are assumed with diameter 0.28 nm, whereas capillary and gel pores distribution range from nanometers to micrometers, which are described by a Raleigh-Ritz distribution function. Considering mass conservation, water transport equation is as follows

$$\rho \left(\sum \phi_i \frac{\partial S_i}{\partial \mathbf{P}} \right) \frac{\partial P}{\partial t} - div(K_v \nabla P) + \rho \sum S_i \frac{\partial \phi_i}{\partial t} - W_p \frac{\partial \beta_{chem}}{\partial t} = 0 \quad (1)$$

Where, *t* is time. *i* represents capillary, gel or interlayer pores, and ϕ_i is porosity. ρ is water density. S_i is pore saturation. *P* is water pressure and ∇P represents its gradient. K_{tr} is water conductivity relevant to porosity and size distribution. β_{chem} is chemically bound water ratio and W_p is cement weight per unit volume.

The first term in Eq. 1 represents pore water capacity. Under an arbitrary relative humidity (RH) meniscus is generated due to water surface tension. Hence, pressure difference ΔP across liquid-vapor interface occurs. Assuming pores are cylinder-shaped and vapor pressure is zero, ΔP equals to P in Eq. 1 and can be described as

$$\Delta P = P = \frac{2\gamma}{r_c} \tag{2}$$

Where, γ is water surface tension and r_c is the pore radius where liquid-vapor interface is present. *P*

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can be also written following Kelvin equation.

$$P = \frac{\rho RT}{M} \ln h \tag{3}$$

Where, *R* is gas constant, *T* is absolute temperature and *M* is water molecular mass. *h* is internal RH. Combining Eqs. 2 and 3, the relationship between *h* and r_c is obtained as

$$\ln h = -\frac{2\gamma M}{RT\rho} \cdot \frac{1}{r_c}$$
(4)

Water status in pore structure is shown in Fig. 1. It is assumed that pores smaller than r_c are totally filled by water. Pores larger than r_c are partially filled because of ink-bottle effect. In the pores which are not filled by condensed water, physically adsorbed water exists. The equations of ink-bottle water and physically adsorbed water are omitted. The saturation S_i in Eq. 1 can be calculated by those three portions of water as follows

$$S_{i} = S_{c} + S_{ink} + S_{ads} = \int_{r_{min}}^{r_{c}} dV + \int_{r_{c}}^{r_{max}} f_{r} dV + S_{ads}$$
(5)

Where, S_c is saturation faction of pores smaller than r_c . S_{ink} is saturation fraction of ink-bottle water. S_{ads} is saturation fraction of adsorbed water. r_{min} and r_{max} are minimum and maximum radii. f_r is the coefficient reflecting the ink-bottle effect.

The second term in Eq. 1 represents the flux, which is assumed principally driven by pore pressure gradient ∇P . The water conductivity K_{tr} is calculated by the following equation

$$K_{tr} = \frac{\rho \Phi^2}{50\eta} \left(\int_{r_{min}}^{r_c} r dV \right)^2 \tag{6}$$

Where, η is water viscosity. Besides, the third and fourth terms in Eq. 1 represent the influences of water consumption by hydration and pore-structure development respectively, and they are obtained by the hydration and pore-structure models.

Finally, moisture exchange with ambient, i.e. surface flux is applied to boundary. When concrete is exposed in atmosphere, moisture is exchanged by means of vapor diffusion and internal-ambient RH difference. Therefore, the surface flux q_s is given as

$$q_s = K_s(h_i - h_s) \tag{7}$$

Where, K_s is moisture diffusion coefficient. h_i and h_s are internal and ambient RHs respectively. On the other hand, when concrete is immersed into water, Eq. 7 does not dominate because moisture is exchanged by means of water flow which is caused by internal-surrounding water pressure difference, rather than vapor flow. Therefore, under submerged condition, surrounding water pressure is directly applied to the boundary, and water flux in Eq. 1 is driven by internal-surrounding pressure gradient.



Fig. 1 Water status in pore structure

3. TWO-PHASE ABSORPTION MODEL

3.1 Discussion on capillary suction in cracks

The model introduced in Section 2 mainly deals with water transport in cement matrix. Verifications conducted by drying, wetting and absorption tests have shown that this model is applicable and effective to cement paste and concrete without obvious cracks. As discussed, from another viewpoint when cracks exist water transport is drastically accelerated. A typical example is the absorption of Engineered Cementitious Composites (ECC). ECC is a family of fiber reinforced cementitious composites. Unlike normal concrete, when tensile stress surpasses tensile strength of cement matrix, ECC shows very high ductility and multiple micro-cracks with tens of micrometers width are generated. Even with such small cracks the absorption process of ECC has been found largely accelerated [2]. This is caused by the well-known capillary suction. Crack can be regarded as a capillary tube, and due to surface tension, water ingresses inside at a comparably high speed. Theoretically, if gravity is neglected, the ingression speed increases as the tube radius increases [3], which is also proved by test [4]. Hence, it is not difficult to comprehend that concrete with larger cracks is more vulnerable to harmful agent penetration.

In the original model, according to Eq. 4, the critical radius r_c increase as RH increase, and the pores smaller than r_c are fully filled by condensed water. In other word, during wetting or absorption pores are saturated gradually from the small parts. Thermo--dynamically it is steady state and can be only attained after long time in reality. Since pores in cement matrix are very fine, water transport is slow so can be regards as quasi-steady state. Therefore, the assumption of steady-state in the original model is reasonable and applicable. On the contrary, cracks are several orders larger than pores, so water transport caused by capillary suction is much more significant. It is a transient state, and the treatment based on quasi-steady state in Section 2 is no longer applicable. Fig. 2 indicates the real absorption process. Water ingresses into cement matrix gradually and meanwhile cracks are flood promptly and saturated in short time. Afterwards, cement matrix absorbs water from not only boundary but also cracks. Therefore, it is difficult or impossible to integrate cracks into the current absorption model, because the



Fig. 2 Water absorption in cracked concrete

dominant mechanisms are different. As a better option, in this study the authors attempt to propose a two-phase model which treats cement matrix and cracks separately as shown in Fig. 3. The water absorption of cement matrix follows the original model, whereas that of cracks is simulated based on capillary suction theory. Cracks are assumed smeared in space field and absorption is treated as a continuous flow process driven by capillary suction force and saturation degree gradient of crack. Furthermore, the process that water is absorbed by cement matrix from cracks is simulated.

3.2 Water transport in cracks

First of all, cracks are assumed smeared in space field. Water mass conservation in an infinitesimal volume of crack field in one dimension is described by

$$\rho\phi_{cr}\frac{\partial S_{cr}}{\partial t} - \left(K_{cr}P_{cr}\frac{\partial^2 S_{cr}}{\partial x^2}\right) + W_{ex} = 0$$
(8)

Where, ϕ_{cr} is the volume fraction of cracks obtained by width and crack number. S_{cr} is the saturation degree of cracks. P_{cr} is capillary suction pressure and K_{cr} is water conductivity of cracks. W_{ex} represents water absorption rate from crack by cement matrix. The first term in Eq. 8 is water capacity of cracks, and the second one is the flux term. W_{ex} is sink term. Eq. 8 represents the one dimension transport for one-direction cracks, and it is easy to be expanded to multi-direction cracks in the future.

As discussed in Section 3.1, capillary suction in cracks is transient state and suction pressure P_{cr} remains constant. Hall summarized transport theories of water flow in concrete, and pointed out that capillary suction is unsaturated flow and can be described by capillary diffusivity and gradient of saturation degree [5]. Accordingly, flux term in Eq. 8 is driven by saturation degree gradient of cracks. In other words, water flows from high saturated part to low saturated part. It needs to be emphasized that this is different from pressure gradient ∇P in Eq. 1 which is used for steady state. The flux q_{cr} driven by saturation degree gradient can be written as follows

$$q_{cr} = K_{cr} P_{cr} \frac{\mathrm{d}S_{cr}}{\mathrm{d}x} \tag{9}$$

Assuming cracks as capillary tubes, similar with



Fig. 3 Scheme of two-phase transport model

Eq. 2, the capillary suction pressure P_{cr} is expressed as

$$P_{cr} = \frac{2\gamma}{w_{cr}} \tag{10}$$

Where, w_{cr} is the crack width. According to the past research [3], water conductivity K_{cr} increases as capillary tube radius increases, and thus can be expressed as the equation

$$K_{cr} = \frac{K_0 w_{cr}^2}{8}$$
(11)

Where, K_0 is the intrinsic conductivity.

Finally, surface flux q_{cr_s} in the boundary where cracks contact water is given as

$$q_{cr_{s}} = K_{cs} \cdot (S_{cr_{s}} - 1.0) \tag{12}$$

Where, S_{cr_s} is surface saturation degree of cracks and K_{cs} is capillary suction coefficient at surface.

3.3 Water supply from crack to cement matrix

Water transport itself in cracks in Section 3.2 is not nonlinear if crack property does not change. In contrast, water supply from cracks to cement matrix is much more complicated because of wide distribution of pore size. Most of micro-pores lie in the range below micrometres, while cracks are much larger in dimension and usually beyond tens of micrometres at least. Therefore, in the proposed model, cracks are assumed as reservoirs in which pores of cement matrix remain absorbing water by means of capillary suction. As suggested by Htut et al [4], assuming an individual pore as a cylinder tube, the distance of water ingression l_w is proportional to square root of radius r and time t, and can be expressed as the equation

$$l_w = K_{cm} \sqrt{\frac{\gamma}{2\mu} rt}$$
(13)

Where, μ is the water viscosity and K_{cm} is non-dimensional mean friction factor. Since pores with various radii contact water simultaneously, according to Eq. 13 it can be deduced that water ingress into coarse pores faster. Fig. 4 shows the image of absorption process by an oven-dried pore structure from cracks. Coarse pores absorb water and become saturated faster than fines ones. According to Eq. 13 and pore distribution, this process can be quantified.

In the pore-structure model of DuCOM, pores are described by a distribution function rather than a series of discrete pores, so discretization according to radius is necessary. Additionally, in most cases the pore structure is not oven-dried, so the condensed water before absorption needs to be considered. The scheme is shown in Fig. 5. Since pores smaller than r_c have already fully saturated, absorption from crack in those pores does not occur any more. On the other hand, pores larger than r_c are only partially saturated and absorption occurs. Referring to Eq. 13, at an arbitrary radius r larger than r_c the increment of absorbed water length d_w can be obtained as follows

$$dl_w = \frac{\alpha K_{cm}}{2} \sqrt{\frac{\gamma t}{2\mu r}} dr$$
(14)

Where, α is effective absorption coefficient relevant to saturation degree of cracks and currently assumed as

$$\alpha = \max(0, 1.25 \cdot (S_{cr} - 0.2)) \tag{15}$$

Eq. 15 implies that absorption rate increases as crack saturation increases. When crack saturation is less than 0.2, absorption stagnates. Still assuming pores are cylinder-shaped, so the available increment of water volume dV_{w1} is obtained

$$\mathrm{d}V_{w1} = \pi r^2 \mathrm{d}l_w = \frac{\pi \alpha K_{cm}}{2} \sqrt{\frac{\gamma t}{2\mu}} r^{3/2} \mathrm{d}r \tag{16}$$

It needs to be pointed out that because of space limitation, the summation of existing water and absorbed water at *r* cannot surpass the total porosity at *r*. In other words, the absorption stagnates when those pores reach saturated. Hence, the real water increment dV_w is as follows

$$dV_w = \min(dV_{w1}, dV_{w2})$$
(17)

Where, dV_{w2} is the remaining volume for capillary absorption. By subtracting ink-bottle water and original physically absorbed water at r, dV_{w2} can be calculated. Finally, by integrating absorbed water in pores larger than r_c , the total absorbed water is obtained

$$V_w = \int_{r_c}^{r_{max}} \mathrm{d}V_w \tag{18}$$

Numerically Eq. 18 can be discretized in time field and the increment during time interval Δt is calculated. Hence W_{ex} , i.e. absorption rate in Eq. 8 is obtained and used as sink term of mass conservation in crack. On the other hand, W_{ex} is appended as generation term in mass conservation equation of cement matrix. Therefore, Eq. 1 becomes





Fig. 4 Water supply from crack to an oven-dried pore structure



Fig. 5 Water supply scheme in the proposed model

4. SIMULATION ON WATER ABSORPTION OF CRACKED ECC MATERIALS

With the two-phase model, water absorption of cracked cementitious materials can be simulated quantitatively. In order to check its applicability, absorption test of cracked ECC is adopted in the verification. One reason for choosing ECC is that multi-cracks can be produced under external load, which is close to the assumption of smeared cracks. In addition, cracks of ECC are usually tens of micrometres wide. Because as tube radius decreases capillary suction pressure increases, for those narrow cracks, gravity is no long significant and can be neglected [4].

The absorption test of cracked ECC was carried out by Sahmaran et al [2]. The mix proportion is shown in Table 1. Water-to-binder ratio is 0.27 and replacement ratio of fly ash is 55% by mass. Beams with $355 \times 75 \times 50$ mm were cast. After demolded at the age of 24 d, the beams were moisture cured at 95 \pm 5% RH and 23 \pm 2°C for 7 days. Then they were air-cured at 50 \pm 5% RH and 23 \pm 2°C until 28 days. After that, 4-point bending load was applied to induce multi-cracks. Finally, the beams were cut into $75 \times 75 \times$ 50 mm specimens for absorption test. Each specimen has 14 cracks with average width 63 µm. Specimens without cracks were test simultaneously as comparison. The absorption test followed ASTM C1585-04 [6]. The specimens were dried at $80 \pm 3\%$ RH and $50 \pm 2^{\circ}$ C for 3 days. Then one surface of the specimen was immersed into water with depth 3~5 mm, and other sides were sealed by silicone coating (Fig. 6). Mass changes were measured, and absorption rate is evaluated by cumulative water absorbed per unit area, which is defined as mass change divided by the cross sectional area of specimens and water density.

The absorption test can be regarded as one dimension, so line elements shown in Fig. 7 are used in the analysis with the proposed model. Mix proportion, curing and exposing conditions are configured completely the same with the test. ϕ_{cr} is obtained by multiplying crack number and width, and divided by water-contacting length. To ensure precision and convergence, time intervals are set as fine as seconds at the beginning of absorption.





The analytical results of absorption are shown in Fig. 8. The vertical axis represents cumulative water absorbed per unit area, while the horizontal axis shows square root of time. Both the uncracked and cracked cases are compared. For the cracked one, water absorbed by cement matrix and cracks are summed together to obtain the total water content. First, it can be found that for the uncracked one, absorption is relatively low and shows linear increase with square root of time. This phenomenon can be traced well by

the original model. In contrast, for the cracked one, the absorbed water content becomes much higher from the beginning. This tendency can be well simulated by the proposed two-phase model. Except for the portion from cracks, the principal reason is that the absorption of cement matrix is much accelerated with the existence of cracks. This can be clearly observed by comparing the absorbed water of cement matrix with uncracked one.





Fig. 9 shows the saturation degree development of cement matrix along the depth from immersion surface for both uncracked and cracked cases. t = 0represents the time just before immersion. Because the specimens were dried at $50 \pm 5\%$ RH until 28 days, before the immersion the area near surface is much drier than interior. For the uncracked case in Fig. 9(a), water content near surface gradually increases but the process is slow, whereas the internal saturation degrees remain unchanged. On the contrary, for cracked case in Fig. 9(b), except for rapid absorption rate near surface, the internal saturation increases simultaneously. Obviously cracks become shortcut for water ingression into cement matrix, which can be only simulated by the two-phase model.

Finally, the influence of crack width on absorption rate is investigated by the proposed model. 10 and 0.1 times of the original crack width is adopted, and the analytical results are shown in Fig. 10. It can be found that with wider crack width, total absorption becomes faster. Fig. 10(b) shows absorption rate of cracks and cement matrix respectively. Obviously the acceleration can be attributed to faster absorption of wider cracks, and correspondingly the process in cement matrix is accelerated. However, the precision needs to be further checked, so in the future more absorption tests with varied crack width are necessary. The influence of gravity on wide crack width is also need to be considered in the future research.



Fig. 10 Absorption analysis with varied crack width

5. CONCLUSIONS

With the existence of cracks in cementitious materials, the absorption process when immersed into water is greatly accelerated. In order to simulate this phenomenon, a two-phase absorption model treating absorption process of cement matrix and cracks separately is proposed. The absorption of cement matrix follows the original model, and water transport is dominated by thermodynamic equilibrium and pressure gradient. On the other hand, water transport in cracks is transient state and simulated based on capillary suction theory. As to water exchange from crack to cement matrix, cracks are assumed as reservoir and keep supplying water. This process is quantitated also by capillary suction theory. The proposed model is verified by absorption tests of cracked ECC. The phenomenon that absorption rate is much accelerated due to the existence of cracks can be well simulated.

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