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Numerical simulation of hydration-driven moisture transport in bulk and interface paste in hardening concrete

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Abstract

In real concrete two types of cement paste can be distinguished, i.e., bulk paste and interface paste. Initially the paste in the interface zone will generally contain more water than the bulk paste and will therefore hydrate differently. Differences in relative humidity and associated differences in pore water pressure will result as well. If the interface paste and the bulk paste could hydrate individually, a situation will result where a relatively porous water-rich interfacial zone coexists with a relatively dry bulk paste. However, due to gradients in porosity, permeability, relative humidity and pore water pressure, a flow of moisture will start from the water-rich interfacial zone to the bulk paste. It will be shown how the moisture transport can be simulated numerically and how this transport phenomenon influences the overall rate of hydration of cement in concrete. Numerical results are compared with experimental data presented in literature. The relevance of modelling of this kind of transport phenomena is briefly dealt with. © 2001 Elsevier Science Ltd. All rights reserved.

Keywords: Hydration; Permeability; Interfacial transition zone; Diffusion; Transport properties

1. Introduction

High-performance concretes are often made with a low water/binder ratio. These increasingly used concretes are susceptible to self-desiccation. This self-desiccation is considered as the mean reason for autogenous shrinkage of low-water/binder-ratio concretes. A very practical and efficient way to reduce the autogenous shrinkage is the use of saturated lightweight aggregate particles in the concrete [1]. These aggregates act as reservoirs, which release their water when the relative humidity in the hydrating bulk paste begins to drop (self-desiccation). It was assumed that, on a less pronounced scale, a flow of moisture will also occur from a water-rich matrix–aggregate interfacial zone to the hydrating bulk paste. The spherical water-rich interfacial zone around a non-porous aggregate particle, shown schematically in Fig. 1, has the same water-supplying function as the saturated aggregate particles in lightweight aggregate concrete. The reason for the flow of water from a water-rich zone to an area with less water is the hydration process, of which the rate depends on the initial local water/cement (w/c) ratio. On its turn, the flow of water from the water-rich interfacial zone to the drying bulk paste will change the effective w/c ratio and hence the local rate of hydration. Direct experimental observation of this hydration-driven moisture flow is very difficult, if possible at all. As an alternative, numerical simulation of moisture flow can be considered. In the following emphasis will be on the moisture flow within ribbon paste, i.e., the paste between aggregate particles.

For the numerical evaluation of hydration-driven moisture flow, information is required about the rate of hydration, the evolution of the pore structure, the relative humidity and the pore water pressure. Absolute values of these quantities are needed, as well as their changes with place and time. In this study, a quantification of the hydration process and the associated microstructural development is performed by the use of the numerical simulation model HYMOSTRUC [3]. In this model hydrating cement grains are considered as gradually expanding spheres. Expansion occurs as the result of

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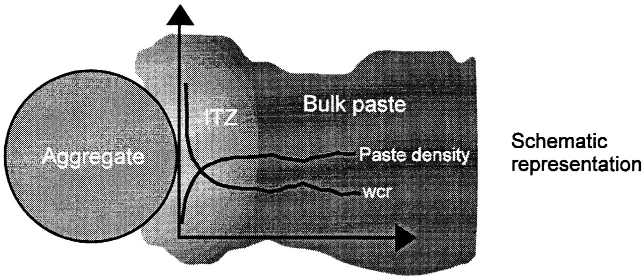

Fig. 1. Schematic representation of matrix–aggregate interfacial zone [2].

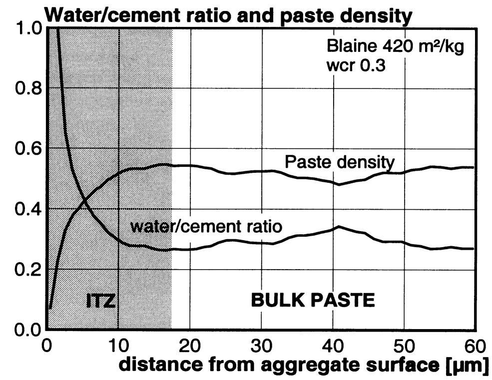

Fig. 3. Local water/cement ratio versus distance from aggregate surface for a paste. Blaine 420 m^2/kg, w/c = 0.30 [2].

the precipitation of reaction products on the outer surface of the hydrating grains. The expanding spheres make contact with adjacent particles and build up a spatial microstructure. The model keeps track of changes in the microstructure, i.e., the pore structure, the amount of capillary water and the relative humidity in the pore system. By using the Kelvin equation, which relates the pressure in the pore water with the pore size and the relative humidity, changes in the pore water pressure can also be followed [2].

2. Ribbon paste hydration

The starting point for a HYMOSTRUC simulation is the spatial distribution of the cement particles in the paste. Cement particles can be placed randomly in a spherical or tubular space (Fig. 2). To analyse the hydration process and moisture flow in ribbon paste, the tubular paste volume is most suitable. The calculated w/c ratio and paste density as a function of the distance from the surface of a solid wall (i.e., an aggregate particle), according to the HYMOSTRUC simulation model for a cement paste with w/c ratio = 0.3 and a Blaine fineness of 420 m^2/kg, is shown in Fig. 3. Due to the less dense packing of cement particles in the interfacial zone, the local w/c ratio there substantially exceeds the nominal mean value.

3. Numerical simulation of hydration-induced moisture transport in ribbon paste

For determination of the progress of the hydration process and hydration-driven moisture flow in ribbon paste, the ribbon is subdivided in small elements (Fig. 4). Each element has a specific initial w/c ratio. For each of these elements, the simulation program HYMOSTRUC calculates the evolution of the hydration process. Due to the differences in initial w/c ratios of the elements, the rate of hydration, the pore structure, the relative humidity and the pore water pressure will be different as well. Pressure gradients in the pore water will trigger a moisture flow from the water-rich interfacial zone towards the “drying” bulk paste. Mathematical details of the transport mechanism are described in Ref. [2]. From the formularies we mention the formula for transport of water:

$$\frac{1}{V}\frac{\partial V_w}{\partial t} = \frac{\partial}{\partial t}\left[\frac{k_w}{\gamma_w}\frac{\partial p_w}{\partial x}\right]$$

where V_w is the volume of water, $k_w(x)$ the local water permeability, γ_w the density of water and $p_w(x)$ the local

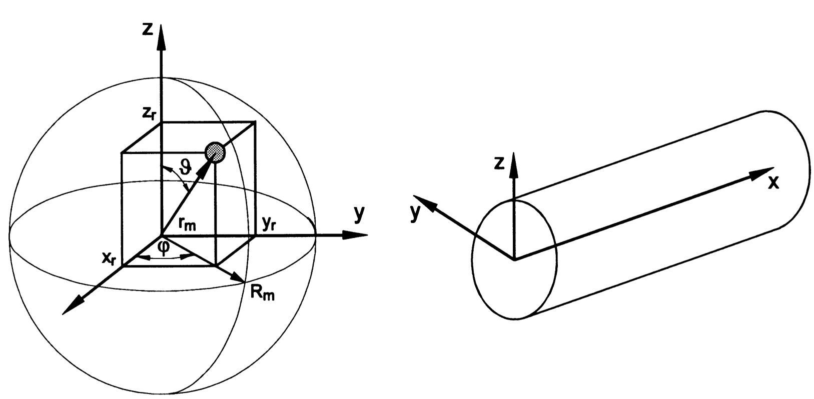

Fig. 2. Random particle distribution in spherical and tubular paste volume [2].

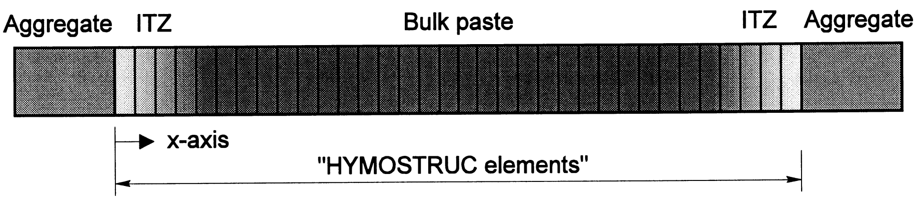

Fig. 4. Proposed model for calculation of hydration and microstructure in the interfacial zone.

pore water pressure. For the consumption of water due to hydration the following equation holds

$$\frac{1}{V}\frac{\partial V_w}{\partial t} = -\frac{0.4\rho_{ce}}{\rho_w + \rho_{ce}\omega_0}\frac{\partial \alpha}{\partial t}$$

with ρ_{ce} the specific mass of cement, ρ_w the specific mass of water, ω_0 the local w/c ratio and α the local degree of hydration. The hydration-induced moisture flow affects the rate of hydration of the bulk paste compared to the situation that moisture transport would be ignored. The moisture flow will depend on the hydration-induced gradients in moisture, water pressure and permeability of the paste.

4. Results of numerical simulations

4.1. Permeability of ribbon paste

The water-rich interfacial zone will result in a higher porosity and a higher permeability compared to the porosity and permeability of the bulk paste, even though most of the cement in the interfacial zone will be converted into hydration product very soon. For a paste with cement with Blaine = 420 m^2/kg and w/c ratio 0.3, the calculated permeability for water and gas over the ribbon thickness of 100 μm after 10- and 100-h hydration is presented in Fig. 5. The high permeability at the aggregate surface decreases steeply to low values in the bulk paste.

4.2. Relative humidity in ribbon paste

In Fig. 6 the calculated relative humidity over the ribbon length is presented. If no moisture transport within the ribbon paste is considered the relative humidity after 10- and 100-h hydration will get values as shown with the thick solid lines. If moisture transport from the water-rich interfacial zone to the relatively dry bulk paste is taken into account, the drop of the relative humidity in the bulk paste will be less, as indicated by the thin solid lines. The relative humidity of the pure paste is also shown in the figure. After 100 h the relative humidity in a pure (plain) paste is calculated at 87%. In the case of ribbon paste, the relative humidity would vary between about 100% at the interfacial zone and 73% to 78% in the bulk paste. This higher relative humidity in the bulk paste will have promoted the hydration process. The calculations reveal, however, that even though the degree of hydration in the bulk paste has increased due to the supply of water from the water-rich zone, the drop of the relative humidity in the bulk paste is less than in the case where no moisture transport is considered.

4.3. Degree of hydration in ribbon paste

In Fig. 7 the calculated degree of hydration in ribbon paste is presented after 10- and 100-h hydration for a paste with a w/c ratio of 0.30 and Blaine fineness of 420 m^2/kg. The degree of hydration after 100-h hydration is presented

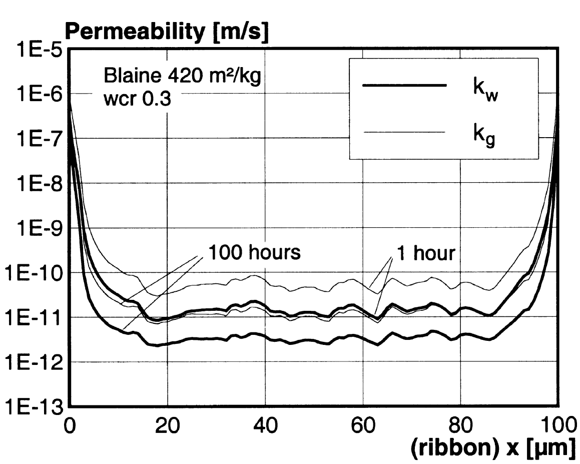

Fig. 5. Water and gas permeability of ribbon paste for a paste with nominal w/c = 0.3 [2].

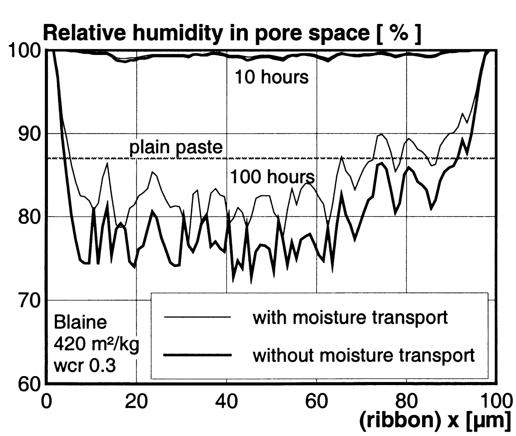

Fig. 6. Calculated effect of moisture transport on relative humidity in ribbon paste and pure paste. Thin line: effect of water transport considered. Bold line: without water transport [2].

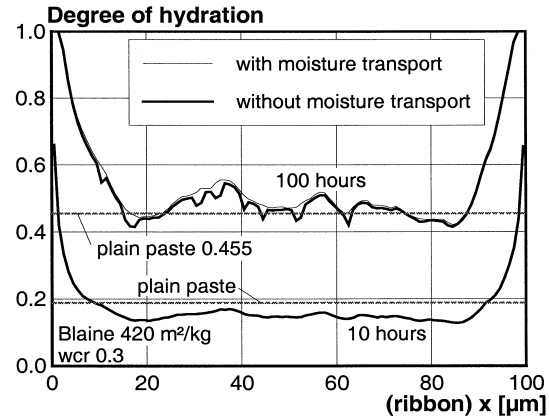

Fig. 7. Calculated effect of moisture transport on degree of hydration over the thickness of a ribbon. Blaine = 420 m^2/kg, w/c = 0.30 [2].

for a calculation with and without taking into account the effect of moisture transport from the interfacial zone to the bulk paste. For this particular mixture, a small increase of the degree of hydration in the bulk paste is found. Compared with the degree of hydration in a plain paste with the same nominal w/c ratio, the ribbon paste has reached a higher degree of hydration. This numerical result is in good agreement with the findings of Roth [6], who mentioned a 10% higher degree of hydration in "concrete paste" than in pure (plain) paste.

5. Discussion and concluding remarks

The strength of cement paste is generally higher than that of mortar and concrete. Walz [4], however, found that under certain circumstances, for example in the case of a mix with a low w/c ratio, the strength of concrete could exceed the strength of the paste. In addition, the use of silica fume can result in strengths higher than the paste strength [5]. An explanation for concrete and mortar strengths close to the strength of the paste is the improvement of the quality of the matrix–aggregate interfacial zone. It is not easy to understand, however, how an improvement of the interfacial zone can ever result in a concrete strength higher than the strength of a paste. An increase of the overall degree of hydration of cement in concrete could be an explanation. In this study the possibility of increased hydration of "concrete paste," i.e., ribbon paste, compared with "pure paste" has been illustrated by numerical simulation. Increased hydration due to the presence of a water-rich interfacial zone as assumed by different authors [6–9] was also found by numerical simulation. In the simulations, an increase of the overall degree of hydration of concrete paste of 5% to 10% was found after 100-h hydration. A similar percentage has been mentioned by Roth [6]. According to Locher [7,8], faster hydration of cement in concrete might be attributed to easier water supply via the porous matrix–aggregate interfacial zone. The results of the numerical simulation presented in this study give support this hypothesis.

It is emphasised that the type of simulations presented here is still in a stage of development. Even in this stage, however, they help to understand the mechanisms behind macroscopic phenomena. The next step is to simulate the effect of saturated lightweight aggregates on the rate of hydration, the relative humidity and associated deformational behaviour of hardening pastes. With the help of a numerical model that is able to quantify moisture flow and associated phenomena, mixture optimisations can be performed in a very efficient way.

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