PREDICTION OF MECHANICAL PROPERTIES AND DURABILITY OF CIVIL ENGINEERING STRUCTURES

Guang Ye (1, 2), Eddy Koenders (1) and Klaas van Breugel (1)

(1) Microlab, Faculty of Civil Engineering and Geosciences, Delft University of Technology, Delft, the Netherlands

(2) Magnel Laboratory for Concrete Research, Department of Structural Engineering, Ghent University, Technologiepark-Zwijnaarde 904 B-9052, Ghent (Zwijnaarde), Belgium

Abstract

This paper reviews the present stage of cement hydration and microstructure simulation program HYMOSTRUC, which was developed at Delft University of Technology, the Netherlands, for simulating the evolution of concrete properties. In the HYMOSTRUC program, cement hydration is simulated as a function of the particle size distribution and the chemical composition of the cement, of the w/c ratio and of the reaction temperature. The program starts from the cement particles size distribution in a 3D body, the cement particles were considered as individual spheres. Based on an "interaction expansion mechanism", the cement grains gradually grow in outward direction. With progress of the reaction process the growing particles become more and more connected. In this way, a virtual microstructure is formed. In this paper, the principle of HYMOSTRUC model are described, the application of this program on the early age properties, the mechanical properties and durability of cementitious materials are presented.

1. INTRODUCTION

In recent years, the performance requirements of concrete structures are continuously challenged. The more and more stringent performance criteria have stimulated fundamental research in concrete technology and structural engineering and have meanwhile brought this on a higher level. It has led to the development of advanced software for the design of concrete structures. Besides this, special software has turned out to be necessary to control the hardening behaviour of concrete, so that a high quality concrete is realized at the "birth" of a structure. Meanwhile the durability of concrete structures is becoming an very important issue to ensure the service life of constructions. Design for 100 years service life buildings brings to the forefront a new challenge to the structural design engineer. Advanced software used for predicting long term properties of concrete structures are certainly required.

Today there are several scientific models such as the NIST model [1, 2], Navi's model [3], HYMOSTRUC [4-7] and Meakawa's model [8], which can be used to simulate cementitious material properties. Each of these models has different specific features and goals. Based on the kinetics of cement hydration, the present HYMOSTRUC program focuses on the microstructure simulation of cementitious materials. This offers a wide opportunity for further development towards a multi-scale model, covering concrete materials from nano-scale, micro-scale to macro-scale (Figure 1). By combining the multi-scale model with existing service life models, and mechanical models, accurate service life predictions can be achieved. The HYMOSTRUC program provides the acceptability of the use of advanced material models in the engineering practice; it will also help to improve the accuracy of models for service life prediction and of macro-scale mechanical models.

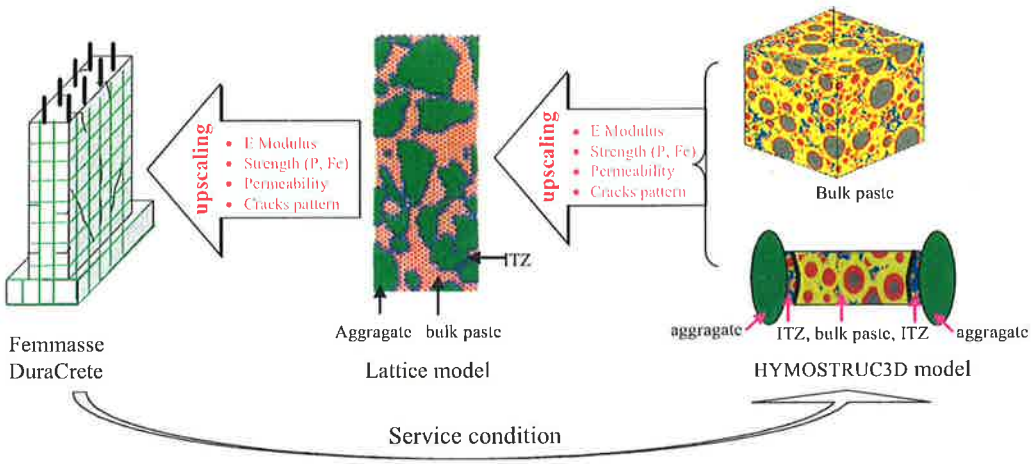


Figure 1: Scheme of multi-scale character of durability problems: Ingress of aggressive species may hurt the quality of the concrete structures

In this contribution the new results will presented generated by the numerical simulation program HYMOSTRUC. Based on the original principle of the HYMOSTRUC model, the program was extended to predict the heat evolution and shrinkage of concrete at early age, the mechanical properties such as compressive strength and tensile strength of cement paste. Based on a simulated capillary pore network, a permeability modulus has been developed. In the paper, the back ground of the HYMOSTRUC model will be provided. It will be shown how a virtual microstructure can be modelled and how mechanical properties can be deduced from it.

2. NUMERICAL MODELLING OF HYDRATION AND MICROSTRUCTURE

2.1. The concept of the HYMOSTRUC model

In the past models for hydrating cement-based systems often focused on either the hydration kinetics or the microstructure. Kinetic hydration models were very much chemistry-oriented. Microstructural models, on their turn, were dominated by physical and stereological considerations. In fact hydration kinetics cannot be considered independently from the

formation of the microstructure. The formation of interparticle contacts, which is the basis of the development of the microstructure, affects the rate of hydration of individual cement particles, particularly in the diffusion-controlled stage of the hydration process.

In principle, HYMOSTRUC model is based on the cell-concept and an associated growth mechanism. In the model a cement particle of a certain size is defined as the central particle of a cubic cell (Figure 2). This central particle, located in the centre of the cube, is the biggest particle in the cell. Going from the surface of the central particle in outward direction small cement particles will be found. When the central particle starts to react and reaction products are formed, this particle will "grow" in outward direction. When grow, small particles will become encapsulated in the growing outer shell (Figure 3).

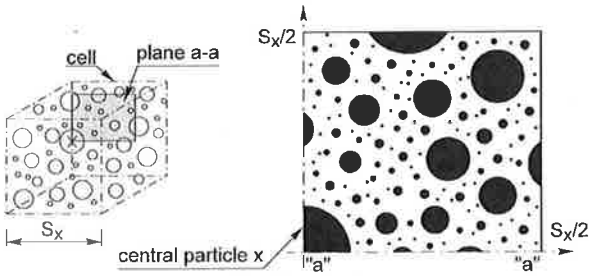


Figure 2: Cell concept adopted in simulation program HYMOSTRUC [4, 6]

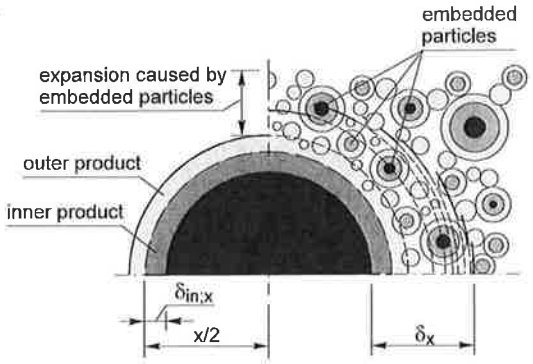


Figure 3: Growth mechanism for central particles with encapsulating smaller particles in the outer shell of the central particle [4].

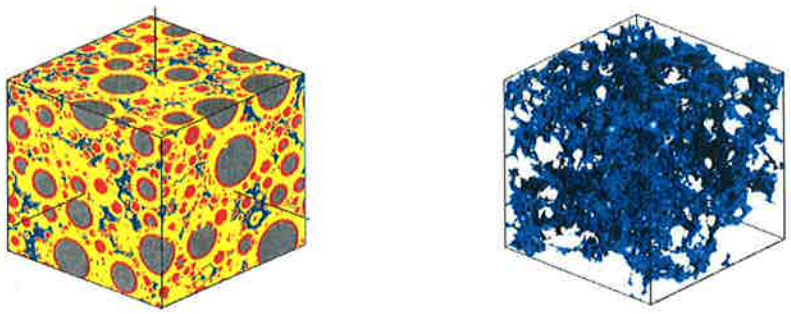
The encapsulated particles may be partly hydrated. If we assume a constant density of the reaction products, the encapsulation of small particles in the outer shell of the growing central particle will create another additional outward growth of the outer shell. This additional growth, on its turn, will result in encapsulating more cement particles and hence in additional growth of the outer shell, etc.. The growth of the central particle, whereby the encapsulation of adjacent particles in the growing outer shell is explicitly taken into account, can be developed in a geometrical series [4]. For each particle in the system the growth process can be determined numerically. With further mathematical manipulations information can be deduced about the amount of cement that is embedded in the outer shell of the central particle. Some of these particles, particularly the bigger ones with a diameter larger than the thickness

of the outer shell, will only partly be embedded in the outer shell of central particle. In principle these particles can become encapsulated in the outer shell of another nearby growing particle as well. In that case these particles form bridges between growing clusters and can give the whole complex of growing clusters its stiffness and strength.

2.2. 3D microstructure generation and analysis

2.2.1 3D microstructure generation

In the HYMOSTRUC model, the cement hydration is simulated as a function of the particle size distribution and the chemical composition of the cement, of the w/c ratio and of the reaction temperature. The model starts from the cement particles size distribution in a 3D body [5], the cement particles were considered as individual spheres. Based on an "interaction expansion mechanism" as shown in Figure 3, the cement grains gradually grow in outward direction. With progress of the reaction process the growing particles become more and more connected. In this way, a virtual microstructure is formed. An example of a simulated cement paste and its pore structure are shown in Figure 4. In the left part the cement paste model is shown, whereas in the right part the accompanying pore structure is presented.



(a). Cement paste (b). Pore structure

Figure 4: Right: Simulated cement paste and, Left: its pore structure with w/c =0.4, at degree of hydration 65%. The physical size of specimen is 100×100×100 μm^3 [7].

2.2.2 3D microstructure analysis

Quantitative description of the geometrical and topological properties of a simulated microstructure is of utmost importance for prediction of the transport properties and mechanical properties. A serial sectioning algorithm associated with overlap criteria was developed within the HYMOSTRUC program as shown in Figure 5. With this technique, it is possible to analyse the connectivity and percolation threshold of the solid phases and pore phases in a simulated microstructure.

The serial sectioning method starts with scanning the 3D microstructure layer by layer. The features of all points in each 2D layer were determined by checking whether an arbitrary point belonged to the subset of the solid phase or to the subset of the capillary pore phase. Secondly, the neighbor points were checked to see whether they are of the same feature, renumber each set with points of the same feature as an individual object (pore or solid). The

information of each object such as coordinate, area and perimeter were recorded. The connectivity of the object between neighbor layers was calculated by an "overlap criterion". The overlap criterion checked each object on its upper-layer and lower-layer to examine whether this object was connected with its neighbors of the same feature. The topological parameter genus was calculated. The volume fractions of the connected solid/capillary pore phase and the total internal pore surface area were derived.

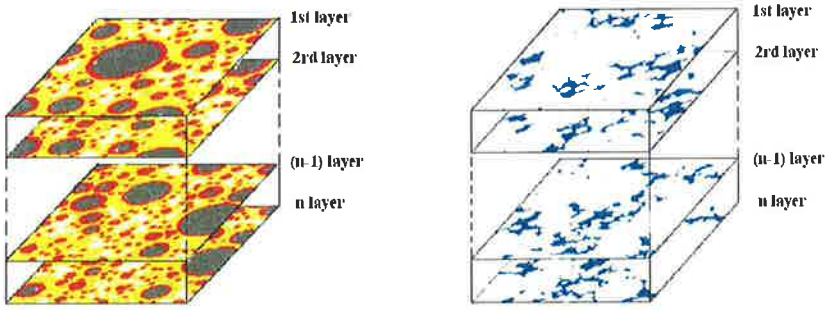


Figure 5: Determination of topological properties by using serial sectioning method and overlap criteria [10].

Figure 6 left shows example where the total porosity and connected porosity are as function of degree of hydration, the sample with water/cement ratio from 0.3 ~0.6, at curing temperature 20°C. The simulation results demonstrate that the water/cement ratio is the most important factor that influences the total porosity and connected porosity. Figure 6 right shows total internal pore surface area as function of degree of hydration.

The characteristic pore size distribution curve can be determined in the following way (see Figure 7).

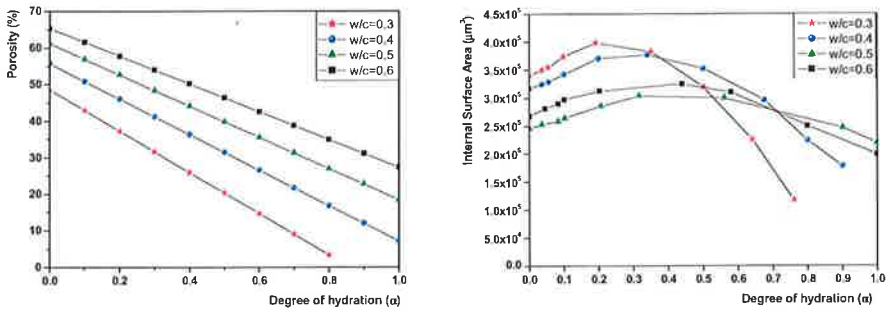


Figure 6: Left: The development of porosity with and, Right: The development of total pore internal surface area, as function of degree of hydration [7].

Consider the sub-volumes of the system accessible to spheres of different radii. Let $\rho_{(r)}$ be the volume fraction of the pore space "coverable" by spheres of radius r. We call these spheres as pore spheres. $\rho_{(r)}$ is a monotonically decreasing function of r and can easily be

compared with the "cumulative pore volume" curves measured by mercury intrusion porosimetry. The derivative $-d\rho_{(r)}/dr$ is the fraction of volume coverable by pore spheres of radius r but not by spheres of radius $r+dr$ and is a direct definition of the pore size distribution. The $\rho_{(r)}$ of the pore spheres with radius r can be computed by densely packing pore spheres in the free space. An example of pore size distribution for cement paste simulated by HYMOSTRUC program is displayed in Figure 8.

are pore spheres with radius as r_1,

are pore spheres with radius r_1+dr_1

are pore spheres with radius r_1+dr_2

Figure 7: The pore size distribution was deterimined by calculting the pore which could be covered by fictition spheres of radius r [7].

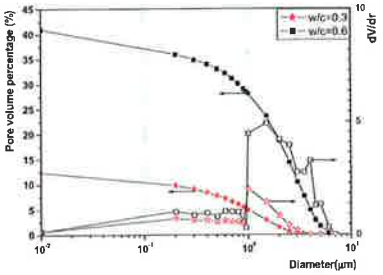


Figure 8: Pore size distribution of simulated cement paste with w/c ratio 0.3 and 0.6 at degree of hydration 0.64. Left axis: pore volume percentage. Right axis: derivative of pore size distribution.

2.3. Modelling hardening shrinkage

Based on the pore size distribution model and the description of the pore volume as provided in the previous section, a shrinkage model could be derived. The model proposed in this section is based on a thermodynamic approach which concept has originally been proposed for hardened concrete by Wittmann [11].

After setting, at a certain stage of the hydration process, pores are partly filled with water. The empty pore volume is filled with water vapour. Based on internal energy balance, a thin layer of water molecules is adsorbed to the pore walls (see Figure 9). There exists a water/vapour interface between the adsorbed water and the air in the empty pores and between the capillary water and the air in the empty pores. In general, this system can be considered as a three phase system, e.g. adsorbed water - interface layer - air (gas). As hydration proceeds, the thickness of the adsorption layer will change. Changes in the thickness of the adsorption layer determine the changes in the surface energy of the gel particles. These changes are accompanied by external volume changes.

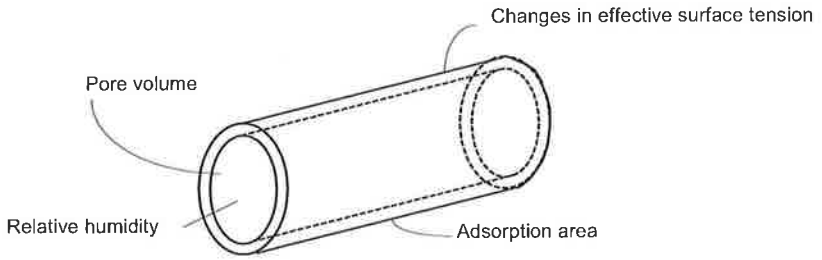


Figure 9: Schematic representation of a pore with an adsorbed layer.

After a proposal by Setzer [12], in this paper only the change of the surface energy at the pore walls of the empty pores will be adopted in the model to describe the thermodynamic equilibrium in the pore system. The capillary surface tension in the dividing surface between the gas phase and the capillary water is not considered. This according to Setzer [12], who gives a detailed motivation for this approach. For the relationship between the changes in the effective surface tension, σ, and the thickness of the adsorption layer $\Gamma(p_g/p_0)$ at a certain relative humidity p_g/p_0, it holds:

$$\sigma = RT \int_{p_g/p_0}^{p_g/p_0=1} \Gamma \, d\left(\ln(p_g / p_0)\right) \tag{1}$$

For a hardening cement paste, the change of the relative humidity in the empty pore space is driven by the hydration process. Since the relative humidity affects the number of mono-molecular layers adsorbed to the pore walls, the surface energy of the hardening cement paste will also be affected. Equation (1), describes the "effective surface energy σ" that remains after the number of mono molecular layers at the pore walls has changed due to a change of the relative humidity in the empty pores. Several authors [11,12], have used different symbols in their papers to indicate this change of the surface energy as described with equation (1). Instead of σ as applied in equation (1), also $\Delta\gamma$ or ΔF are used. All notations are, in fact, applied to describe the same mechanism, viz. the change of the surface energy in the system.

2.4. Shrinkage deformations

It was Bangham [13] who related the external deformation of coal to the change of the surface energy. In several papers [13] Bangham applied the adsorption equation of Gibbs to describe this phenomenon. Bangham used his theory to point out that with solid surfaces, as opposed to liquid surfaces, the surface energy, representing the work spent for the formation of a unit of new surface, must be in thermodynamic equilibrium with the pressure. In his work, he considered a three-phase system as mentioned in the previous sections. He found that the expansion of

coal could be related linearly to changes in the internal surface energy with increasing thickness of the adsorption layer. This approach has been shown to be valid for hardened cement paste by, among others, Wittmann [11]. It is noticed that the Bangham equation has a semi-phenomenological basis and should not be considered as a physical law. This should be born in mind when it is proposed to apply a modified Bangham equation (see e.q. (3)) for quantification of the deformational behaviour of hardening cement-based systems in which the relative humidity is beyond the range considered by Bangham, which was up to about 40%.

When dealing with hardening cement paste, the material properties change continuously with progress of the hydration process. Therefore, the relationship between the external deformation and the changes in effective surface energy must be considered incrementally and can be formulated as:

$$\frac{\partial \varepsilon_a(\alpha(t))}{\partial \alpha} = \lambda \cdot \frac{\partial \sigma(\alpha(t))}{\partial \alpha} \tag{2}$$

where $\partial\varepsilon_a(\alpha(t))$ is the strain increment that describes the microstructural deformation of the hardening paste (autogenous shrinkage due to self-desiccation), $\partial\sigma(\alpha(t))$ the change of the effective surface energy (see eq.(1)) and λ a proportionality factor. In fact, this proportionality factor is the compliance modulus of the hardening material, e.g. cement paste.

Analogue to the Bangham approach, the proportionality factor has been modified in order to be applicable for modelling volumetric changes of hardening cement-based materials. In this respect, the pore wall area requires due attention. As hydration proceeds, pores will be emptied. This implies that a certain part of the pore wall area borders on the capillary pore water (filled pores) and a remaining part borders on gas phase (empty pores). Only the pore wall area of the empty pores has to be considered in the description of the volumetric changes of the adsorption area (see also Figure 6). This is also required from a thermodynamic point of view, since the load that acts on the microstructure from the interior, is exerted by the effective surface tension in the adsorption area [12].

Therefore, the proposed constitutive equation has the following shape.

$$\lambda(\alpha, RH, wcr) = \frac{A_{int}(\alpha) \cdot \rho_{pa}(wcr)}{3 \cdot E_p(\alpha)} \tag{3}$$

where:

$A_{int}(\alpha)$ = internal surface area of the empty pores
$\rho_{pa}(wcr)$ = specific mass of the cement paste
$E_p(\alpha)$ = modulus of elasticity of the cement paste

From constitutive relation (3), it is remarkable that, besides the degree of hydration and the water/cement ratio, the proportionality factor λ also depends on the relative humidity in the empty pore space.

3. APPLICATION OF HYMOSTRUC PROGRAM

The program HYMOSTRUC was used to predict early age properties such as degree of hydration, heating release during hydration, the percolation of phases. Mechanical properties including compressive strength of cement paste. Permeability of cement paste is predicted based on a pore network model. Most recently a new user interface has been developed and a free downloadable limited edition of the Hymostruc model has been put on the website of the Microlab (www.microlab.citg.tudelft.nl).

The base screen of the user interface of the free downloadable limited edition of the Hymostruc model is provided in Figure 10. The interface contains tags to assign the input values for the Binder properties, the Concrete mixture, the 3D particle structure and, finally, a tag to control the calculation process. Two visualisation options are enclosed in the model. These are a graphics module, that show the results of a run and a 3D visualisation module that enables the opportunity to evaluate the generated 3D particle structure. The model enables the opportunity to calculate the degree of hydration and to generate a virtual microstructure of a Portland based cement paste mixture or concrete.

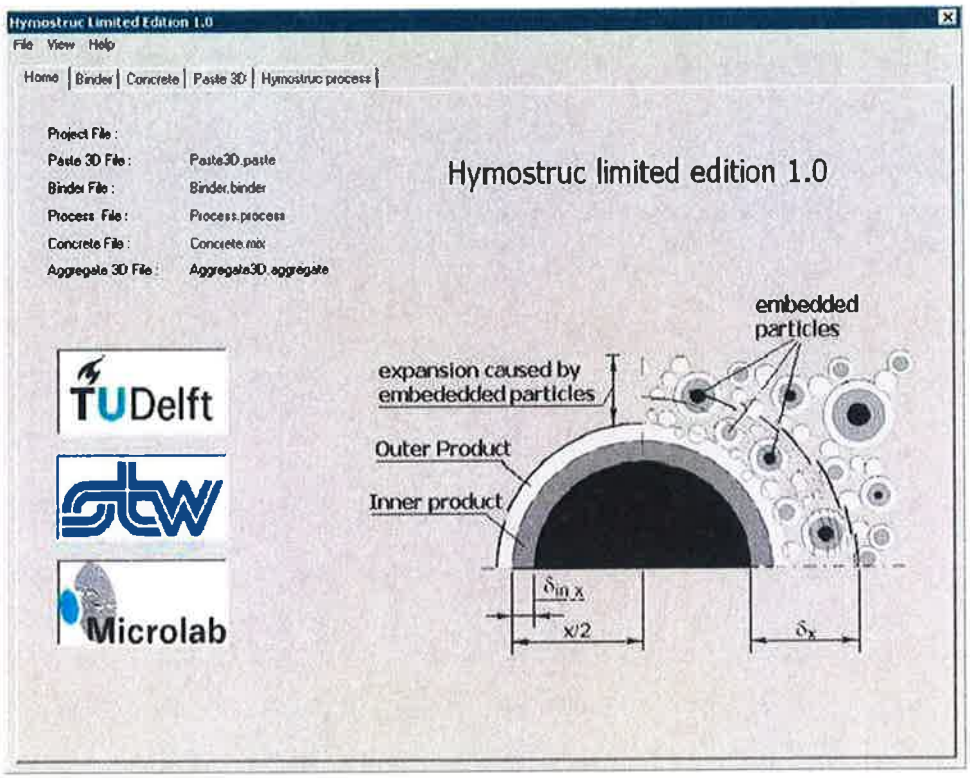


Figure 10: User interface of the free downloadable Hymostruc limited edition.

3.1. Degree of hydration

The evolution of the degree of hydration can be simulated numerically with the HYMOSTRUC model. In a systematic calculation procedure, the increase of the overall degree of hydration is determined by adding up the contributions of the individual particle fractions. These contributions are determined from the progress of the reaction front into the individual cement particles. For the rate of penetration of the reaction front in a cement particle, a *basic rate equation* is proposed [4] in which the effects of the formation of microstructure, i.e. of the interaction between hydrating and expanding particles and the rate of hydration, is explicitly accounted for. The basic rate equation comprises reduction factors that affect the rate of the hydration process. These five factors comprise:

1. The change between phase-boundary and diffusion controlled reaction process.
2. Water withdrawal of particles embedded in the outer shell of larger particles.
3. The effect of the distribution of capillary water in the pore system.
4. The amount of capillary water in the pore system.
5. The effect of curing temperature on the rate of penetration of the reaction front

With the basic rate equation, the volume of hydration products which are formed on a micro-scale level can be determined. In order to obtain information about the actual state of the hydration process, the volume of hydration products must be related to the total volume of cement that is available in the cement paste. The rate at which the hydration products are formed depends on several parameters. In this respect, two dominant parameters are the particle size distribution and the water/cement ratio. In the HYMOSTRUC model, the influence of these parameters on the rate of the hydration process is dealt with explicitly.

For a plain Portland cement paste, the influence of the fineness of the cement and the water/cement ratios on the degree of hydration is shown in Figure 11. The cement type with the highest fineness shows the highest rate of hydration.

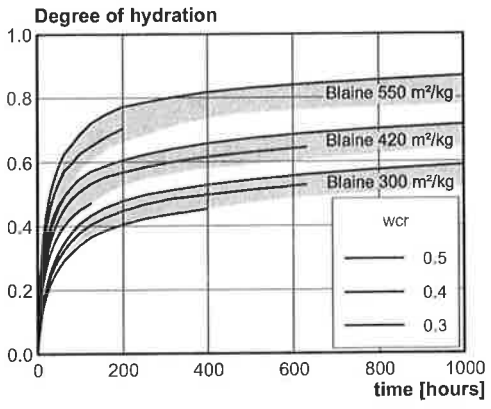


Figure 11: Calculated degree of hydration for different cement finenesses and wcr's.

3.2. Autogenous shrinkage versus relative humidity

The degree of hydration reached at ceasing of the hydration process is lower for the cement pastes with a lower water/cement ratio. Too little water is available to proceed whit the hydration process. For low water/cement ratio pastes(e.g. wcr 0.3) the maximum pore diameter of capillary pores that are still completely filled with water is much smaller than the maximum pore diameter of a cement paste with a higher water/cement ratio (e.g. wcr 0.5). This phenomenon will result in a lower relative humidity in the emptied pore space and introduces a larger change of the surface energy and, finally, it results in larger deformations of the microstructure (eq. (1) and (3)). The thermodynamic equilibrium in the pore system governs this process.

This mechanism shows that autogenous shrinkage on the one hand, depends on the amount of water available in the system expressed in terms of the water cement ratio and, on the other hand depends on the fineness of the pore structure. This is the reason that no limiting water cement ration can be proposed beyond which no autogenous shrinkage will occur anymore because the fineness of the pore structure in this approach is still undetermined. This means that autogenous shrinkage might also occur for mixtures with for example a water cement ratio of 0.5 in combination with a cement of high fineness. This result has also been confirmed experimentally (see Figure 12, right). The results in this figure shows the autogenous shrinkage measured for cement paste (Portland cement) for three different water cement ratios, i.e. 0.3, 0.4 and 0.5. The results show significant shrinkage for all three pastes. The major difference is caused by the rate at which the shrinkage develops. The paste with the lowest water cement ratio shows the highest rate at which the shrinkage develops. The paste with the highest water cement ratio shows the opposite behaviour.

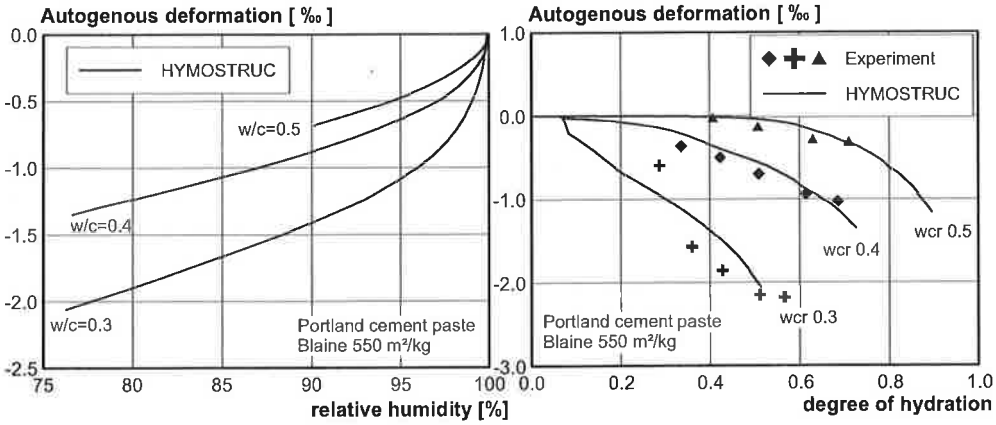


Figure 12: Left: Hardening shrinkage autogenenous versus relative humidity in the empty pore space (self-desiccation); Right: Autogenous deformation for different water cement ratios and a cement fineness of 550 m^2/kg.

3.3. Percolation of capillary porosity and solid phases

The percolation theory deals with disordered multiphase media in which the disorder is characterized by the degree of connectivity of the phases. In percolation studies one is often interested in the fraction of a phase, which is connected across the microstructure as a function of the total volume fraction of the phase. In particular, the de-percolation of capillary porosity is of great interest for studying the transport phenomena in cement-based materials.

Figure 13 shows results of the percolation threshold of the solid and capillary porosity for two different w/c ratios. The solid percolation threshold was found at a degree of hydration 0.02 for w/c ratio 0.3 and at a degree of hydration 0.025 for w/c ratio 0.4. Afterwards, the connected solid phase shows a quick increase and all solid particles are connected at a degree of hydration of 0.25 for both w/c ratio samples. For the evolution of the capillary porosity, Figure 9 shows that almost all capillary pores are connected with each other up to a degree of hydration of 0.70. A value of 3.5% of the capillary porosity percolation threshold is found in both samples, corresponding to a degree of hydration 0.91 for the sample with w/c ratio 0.4 and a degree of hydration 0.63 for the sample with w/c ratio 0.3.

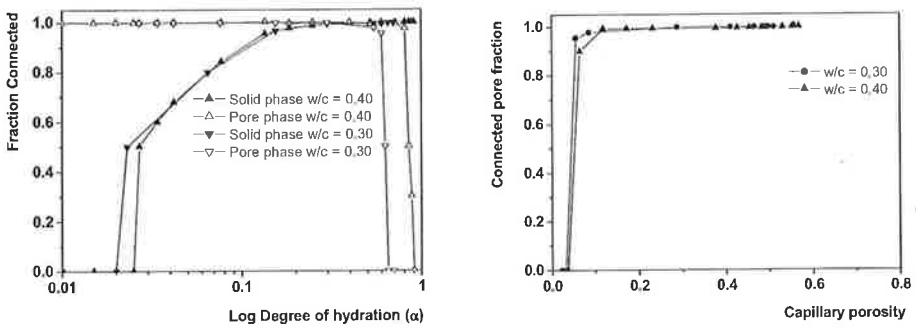
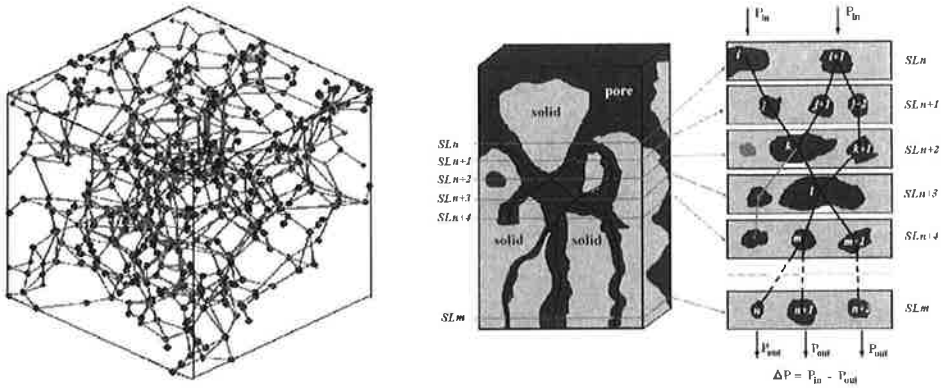


Figure 13: Left: connected fraction of the phases as a function of degree of hydration. Right: connected pore fraction as a function of capillary porosity [14].

3.4. Water permeability prediction

Based on the overlap criterion, a linked list pore network structure can be obtained (Figure 14). From the link list network, the effective hydraulic conductivity is estimated. The fluid flow is calculated according to the Hagen-Poiseuille law. The pressure distribution of all nodes is calculated by applying a conjugate gradient method and the absolute permeability of the pore network is calculated directly from Darcy's law. The detailed description of the algorithm is presented in [15].



a) b)

Figure 14: Schematics of building up the linked list network pore structure and permeability calculation based on a pore network model [15]

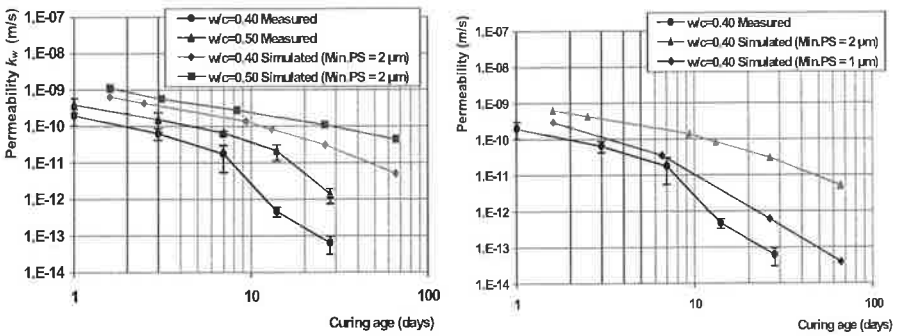


Figure 15: Left: Measured and predicted permeability for two w/c ratio samples in the first 28 days. Right: Predicted permeability (w/c ratio=0.40) influenced by minimum particle size. Error bars indicate the standard deviation of the experiments [15]

In Figure 15 left, a comparison between the measured and simulated values of permeability (minimum particle size 2 µm) is given. The simulated values for samples with w/c 0.40 and 0.50 are 2 or 3 orders of magnitude higher than the measured values. The differences are more pronounced in the later hydration stage. In the case of w/c 0.40, the simulated permeability for the sample with minimum particle size 1 µm is also compared with the measured results, as shown in Figure 15 right. Compared to the sample with minimum particle size 2 µm, the simulated permeability of the sample with minimum particle size 1 µm is much lower and closer to the experimental results. In fact, it is only 1 order of magnitude higher than the measured values in the later stage and very close at early age, up to 7 days.

3.5. Early age compressive strength of cement paste

In cement hydrating system, with the increasing of the hydration time, the cement particles continuously react with water and form hydration products, which precipitate around the unhydrated cement particles. The hydration products are becoming more and more interconnected with each other as the hydration proceeds. The result of this interconnectivity between hydration products leads to a change on the materials properties, for example, the increase of the compressive strength and elastic moduli. In the HYMOSTRUC model, the interconnectivity between hydration products was described based on the concept of contact area [Figure 16].

In the simulation program, it is assumed that the hydration products are the results of a central growth of the original sphere diameter. With the progress of hydration, the diameter of sphere increases and the hydration products will contact each other. The amount of contact area between two or more particles increases with an increase in the degree of hydration. From the equilibrium condition and virtual work principle, the compressive strength P can be calculation as function of total contact area of hydrating cement [16]:

$$P = kD^{-2}(Ac)^{\frac{3}{4}}\sqrt{E\gamma} \tag{4}$$

Where, D: diameter of sphere (μm). Ac is total contact area (μm^2). E is the elastic modulus of particle [GPa], γ is specific surface energy (N/m). *k,* the microstructural parameter related to the amount of CSH and CH during cement hydration.

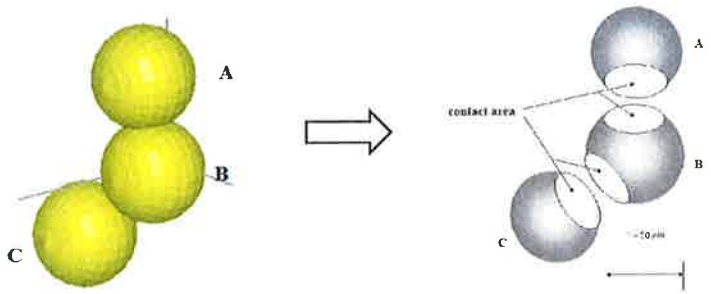


Figure 16: Left: The concept of contact area 3 hydrating cement particles, Right: contact area A_c between particle A, B and C.

An example of the simulated compressive strength of three cement pastes are shown in Figure 17 and compared with experimental results. Regardless the size effect in the compressive strength test, the simulated strength at later age shows a good agreement with experiments.

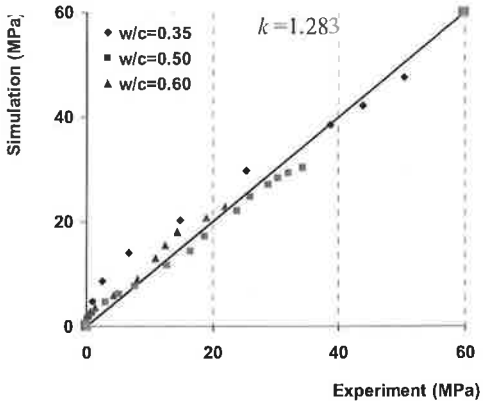


Figure 17: The comparison of compressive strength of three cement pastes between simulation and experiments [16]

4. CONCLUSIONS

In this paper, the principle of numerical simulation program HYMOSTRUC is presented. The advantages of this program were taken into account the kinetics of cement hydration and stereology of cement particles packing. Based on the simulated virtual microstructure of cement paste, this paper shows that the program is able to predict the properties of cementitious materials, like the early age properties, (degree of hydration, autogenous shrinkage et. al); and the permeability and compressive strength of cement paste. Percolation theory was applied to study the transport properties of cementitious materials.

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