MODELLING OF THE HYDRATION OF HIGH PERFORMANCE CONCRETE WITH NORMAL- AND LIGHTWEIGHT AGGREGATES

MODELLIERUNG DER HYDRATATION VON HOCHLEISTUNGSBETON MIT NORMAL- UND LEICHTZUSCHLAG

MODELISATION DE L'HYDRATATION DU BETON AVEC LES AGREGATS NORMAUX ET LEGERS

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SUMMARY

This article is the continuation of the preceding Otto-Graf-journals essay over DuCOM [1]. The program DuCOM discussed there was extended by the possibility of modelling high-strength concrete containing normal and lightweight aggregates. The obtained results are compared with experimentally determined data.

ZUSAMMENFASSUNG

Dieser Artikel versteht sich als die Fortsetzung des im vorhergehenden Otto-Graf-Journals veröffentlichten Aufsatzes über DuCOM [1]. Das dort diskutierte Programm DuCOM wurde um einen Ansatz zur Modellierung von hochfesten Betonen mit Normal- und Leichtzuschlägen erweitert. Die erzielten Rechenergebnisse werden mit experimentell ermittelten Daten verglichen.

RESUME

Cet article est la continuation de l'essai du DuCOM qui a été publié dans le Otto-Graf-journaux précédent [1]. Le programme DuCOM, discuté dans ce journaux, a été ajouté à la possibilité de modeler un béton de haute résistance contenant les agrégats normaux et légers. Les résultats obtenus sont comparés aux informations expérimentalement déterminées.

KEYWORDS: DuCOM, simulation of concrete hydration, high strength concrete

1. INTRODUCTION

High performance concretes are concretes fulfilling highest claims in regard to their properties. The best known high performance concrete is the high strength concrete. A crucial characteristic of high strength concrete is its low water-paste ratio. The workability of concrete with low water-paste ratio became possible due to the invention of concrete fluidisers and fluxing agents. It was proven theoretically that an ordinary Portland cement concrete with a water-paste ratio of 0.36 that was stored under water can completely hydrate and no capillary pores will develop. The water-paste ratio of a high strength concrete amounts up to 0.30. This is less than the value that is necessary to provide complete hydration. Hence the danger of self-desiccation exists with developing hydration if no additional water will be provided. Furthermore high strength concrete develops within the first days such a dense structure that no water from the outside can infiltrate into the structure. Because of this effect all common after treatment methods of concrete are ineffective and the self-desiccation occurs resulting in early age shrinkage and cracks inside the structure do emerge. The strength development stagnates due to the crack initiation. An inside water reserve that is provided by water saturated light weight aggregates can help to avoid these effects. During a testing program of the IWB concretes were produced with normal and light weight aggregates [3;4]. It was found that water saturated light weight aggregates were functioning as additional water reservoir inside the concrete and that they were fulfilling the function as an after treatment for concrete. Without any outside after treatment the concretes with 25% light weight aggregates content reached a 20% higher strength after one year compared to concretes with solely normal weight aggregates. In comparison to normal weight concrete there weren't any visible cracks found at specimens with light weight aggregates and the slump of the 180 days strength of normal weight concrete failed to appear. These attributes of high strength concrete should be simulated and attributes relevant for construction sites like compressive strength should be predicted by the computer model. The used model is based on the DuCOM [2].

2. PRINCIPALS

The Liapor F8 grains have a grading curve where a 88% fraction remains between the sieve sizes of 4 and 8 millimetres. Hence the average diameter was assumed with six millimetres. This assumption results in a globe volume of 113.09 mm^3. This volume was converted to an equivalent sized cuboid having an edge length of about 4.8 mm. It was necessary to use cuboids because Du-COM is only able to calculate with eight nodes elements. In dependence of the fraction of Liapor of the concrete mixture the size of the surrounding concrete matrix was calculated. The names of the simulated cubes and mixtures refer to the proportion of light weight aggregates in the mixture. The used mixtures are given in Table 1.

Table 1: Used mixtures

	HB 0	HB 15	HB 25	HB 30
light weight aggregate [vol.-%]	0	15	25	30
w/c-value	0,33	0,33	0,33	0,33
cement [kg/m^3]	450	450	450	450
fine aggregates [kg/m^3] fraction ≤ 4/8	815	737	691	689
coarse aggregates [kg/m^3] fraction ≥ 4/8 without light weight aggregates	934	800	524	449
light weight aggregates 4/8 [kg/m^3]	0	212	534	611
17% water content of the light weight aggregates [kg/m^3]	0	36,04	90,78	103,87

During all simulations the used boundary conditions were for the first three days constant. The temperature was 20 degrees Celsius and humidity 100%. After this time the humidity was reduced to 65%. The temperature remained constant. The Liapor grain was modelled as a concrete mixture that has a very high water content, a very low cement content and no other supplements. Thereby a sufficient water content and a relatively low strength were achieved.

This approach was chosen because DuCOM can't simulate any other materials except of concrete.

3. IMPLEMENTATION OF LIGHTWEIGHT AGGREGATES

The theoretical description of light weight aggregates assumes an ideal dispersion of light weight aggregates within the concrete mixture [2]. If the aggregate content is below a certain fraction there won't be a continuous network with a porosity that is high enough to build up continuous pores. Because of this the problems of moisture exchange can be reduced to the interactions of grain and surrounding matrix. Light weight aggregates can be simply described as a water reservoir with certain attributes in regard to water content and strength. Therefore it can be described as :

$$\frac{q_{fl}^{ag}}{t} = R_{cap.-\ agg,} + R_{matrix.-\ agg.}$$

q_{Fl}^{Ag} : water content of the light weight aggregates

$R_{cap.-\ agg.}$: speed of water delivery to the capillary pores

$R_{matrix.-\ agg.}$: speed of water delivery to the concrete matrix

The water content of aggregates can be calculated by considering the saturation of the pores with any fluid. The water vapour content can be neglected.

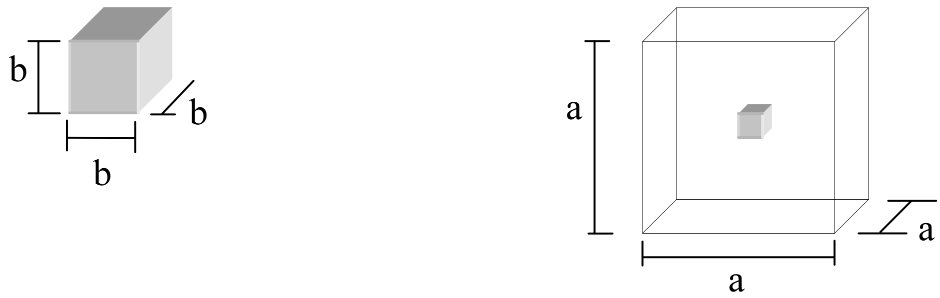
$$q_{Fl}^{Ag} = r_{Fl} f_{Agg.} S_{Fl.}$$

r_{Fl} : density of a fluid; $f_{Agg.}$: porosity of aggregates;

$S_{Fl.}$: saturation of aggregates

The results of the performed simulations have been achieved by a different approach. The light weight aggregates have not been part of the mathematical description of the concrete matrix. They were modelled as an element with the attributes of water saturated aggregates. Two types of models were created for the simulations. One with a dense mesh for simulations of the dispersal of moisture within the concrete (figure 3) and another one for the calculation of compressive strength and degree of hydration. Therefore it was necessary to use a coarse mesh (figure 2) otherwise computing time would have been very high. The size of the light weight aggregate has been constant while the thickness of the concrete matrix differed in dependence of the proportion of light weight aggregate (figure 1). For each model three simulations were performed. One to simulate an adiabatical system; another one with a system where one side of the cube had an exchange of temperature and humidity and the last one where two sides had an exchange with the environment. These boundary conditions were chosen to simulate the inside, a cube placed on the surface of the column and one in the corner having two surfaces.

light weight aggregate: concrete matrix:



with all mixtures:	dimensions :		
b = 4.836 mm	HB 0	a = 9.09 mm	V = 751.2 mm^3
V = 113.09 mm^3	HB 15	a = 9.09 mm	V = 751.2 mm^3
	HB 25	a = 7.67 mm	V = 450.7 mm^3
	HB 30	a = 7.22 mm	V = 375.6 mm^3

Figure 1: Geometry of the simulated cubes

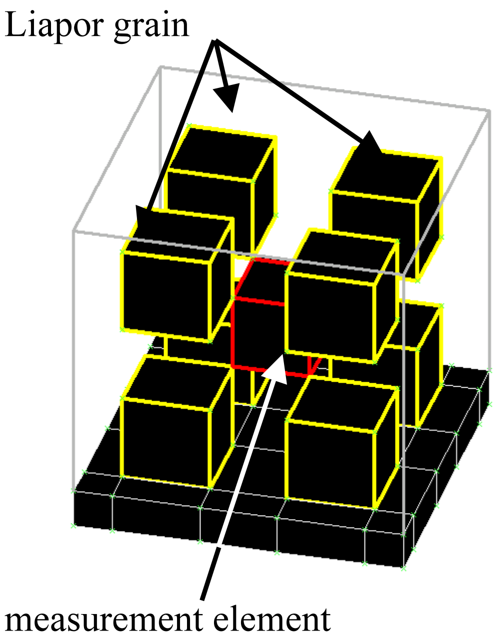


Figure 2: Model with eight Liapor grains

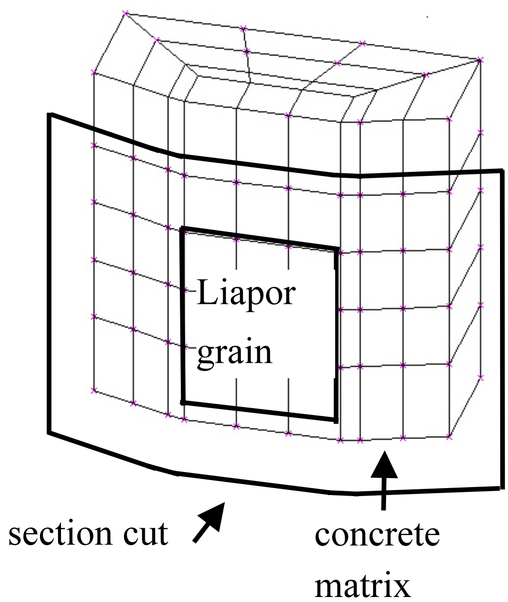


Figure 3: Model with one Liapor grain

4. RESULTS OF THE SIMULATIONS

Degree of hydration

The in figure 4 shown curve-progressions are the results of the simulations of the hydration degree resulting after 365 days of curing. The adiabatical curves are shown as an example for the simulations.

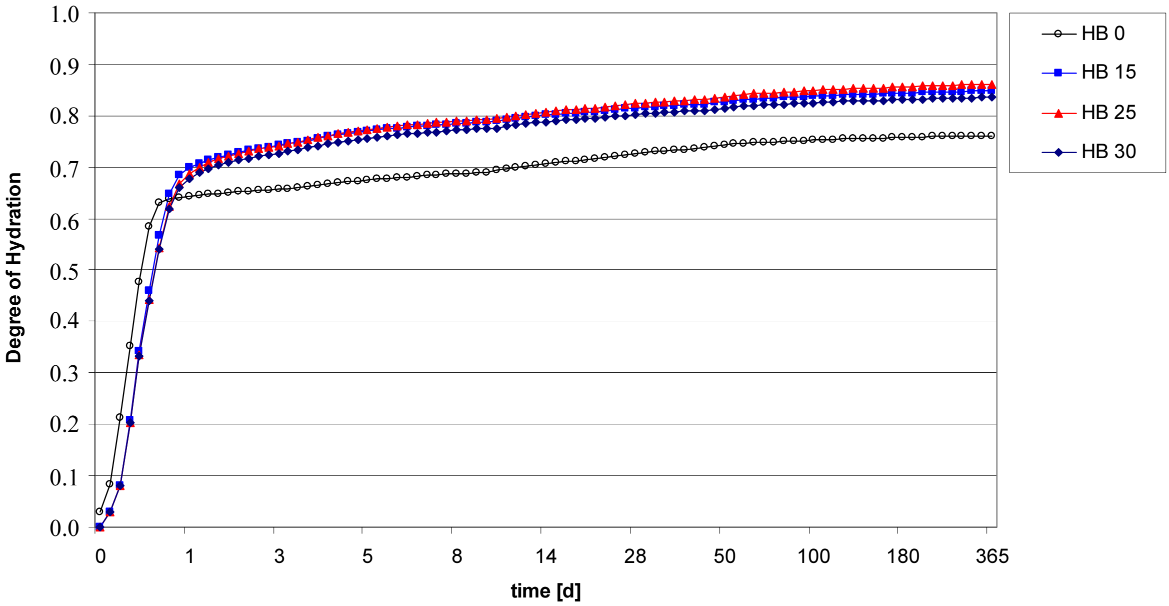


Figure 4: Development of the hydration degree in an adiabatical system

Because the heat loss is circumvented within an adiabatical system the heat increases rapidly. After one day the water loss reduces the reaction speed significantly and the curve growth of the mixture without an additional water reservoir (HB 0) decreases. For the mixtures with water saturated light weight aggregates this effect is postponed. This results in a higher degree of hydration. It can be shown that the hydration continues approximately up to the age of 80 days. Between the 2. and the 80. day the remaining capillary water diffused into the grain through the CSH needles and reacts with the cement. The difference between mixtures with and without light weight aggregates is growing until the 9. day. After this time the gap between HB 0 and the other curves decreases again. This can be explained by the resulting slower reaction because of the bigger grain boundary surface of the higher hydrated mixtures. The mixture HB 25 reaches the highest level of hydration of all mixtures.

To show the influence of the light weight aggregates and the boundary conditions on the hydration degree it was best to provide these information in a single plot. At the age of 14 days the difference between the curves are the biggest. Figure 5 shows the hydration degrees at this age.

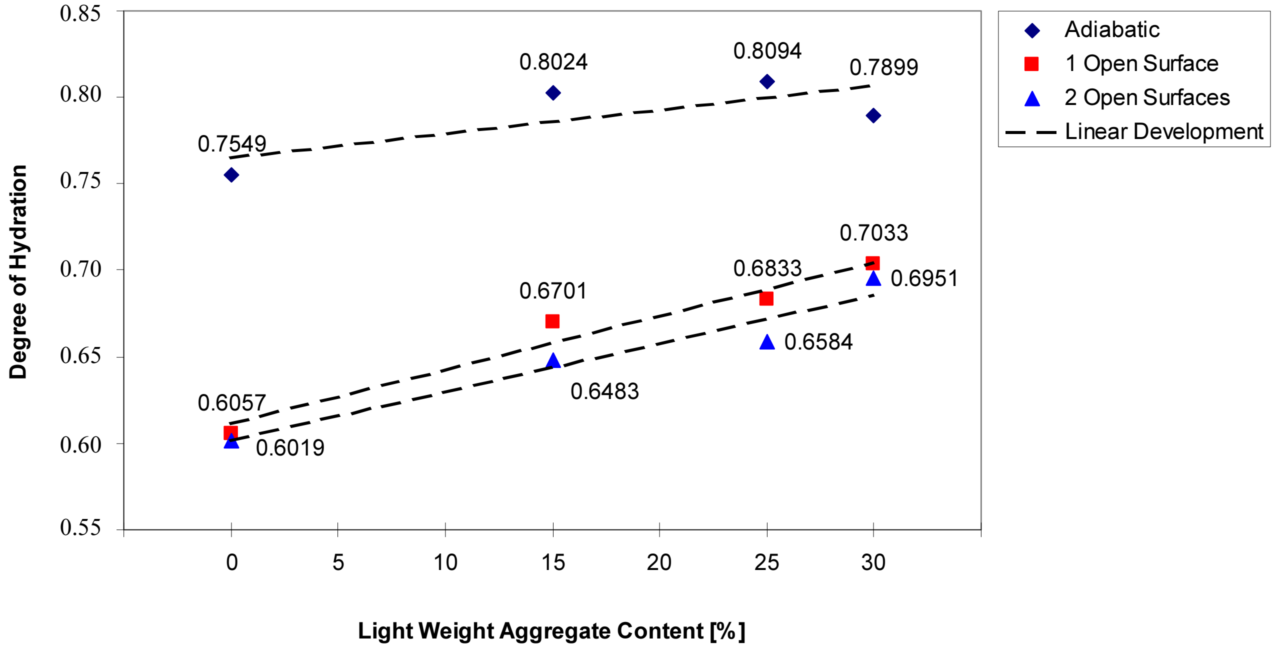


Figure 5: Degree of hydration at the age of 14 days

The influence of the content of water saturated light weigh concrete is clearly visible. With increasing aggregate content the hydration degrees reached are increasing too. The linear development line shows for the simulations with an exchange with the environment a fast ascending slope. The lines for one and two open sides develop approximately parallel to each other. The line for an adiabatical system has a very flat progression. This can be explained by the non existent moisture loss to the environment. All the water of the mixture reacts with the cement and this continues until all the water has been used. One reason why the additional water content has little effect on the hydration degree might be that the water transport mechanism is controlled by Darcy's law which connects local pressure differences with permeability. Hence within an adiabtical system no transport of vapour and water exists. The influence of the additional water is reduced to nodes of elements that are connected with light weight aggregates and the cement matrix. Since the compressive strength is dependent on the hydration degree the curve progressions do resemble each other.

Dispersion of moisture

This picture should provide an impression of the possibilities of the simulations. It shows a plot of the results of the capillary water after 4.2 days. The water content is given in kg/m^3. The cube had one open side that permitted an exchange of temperature and moisture. It was the side the z-axis is directed to.

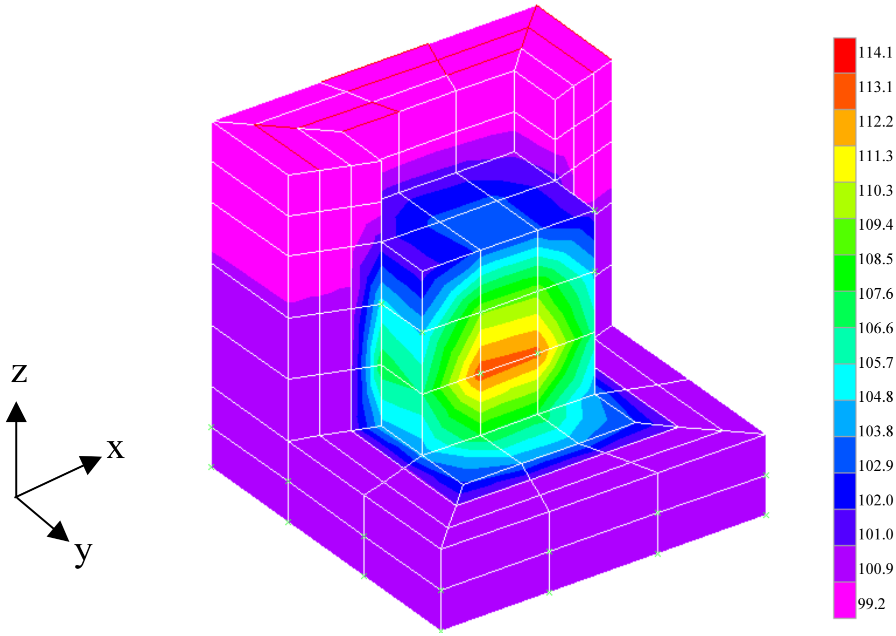


Figure 6: dispersion of humidity simulated with a model as shown in figure 3

The water content in the center of the Liapor core is reaching 113 kg/m^3. This is significantly higher than the moisture content of the surrounding areas. At the free open side the free water content is 99.2 kg/m^3 . The remaining concrete matrix has a water content of 100.9 kg/m^3 while the transition area between the core and the matrix has an average water content of 102.9 kg/m^3. These numbers were measured after 4.2 days. The amount of chemically bound water reached after 365 days 80 to 90 kg/m^3 (Table 2). The water reservoir of the Liapor grain reaches 20 kg/m^3 after one year. The calculated autogenious unrestrained drying shrinkage shows a significant decrease for specimens with water saturated light weight aggregates. Especially if two cubes, one with and one without water saturated light weight aggregate, are compared. The numbers are not corresponding with the measured ones but they do show the same tendency like the in the laboratory gathered results.

Table 2: chemically not bound water of the concrete matrix

mixture	simulation	t=0 d	t=0,15 d	t=360 d
		max [kg/m^3]	max [kg/m^3]	max [kg/m^3]
HB 0	adibatical	150	142	57
	1 open side	150	142	65
HB 15	adiabatical	150	142	72,5
	1 open side	150	142	65

5. DISCUSSION

The calculated results were compared with experimentally obtained numbers. These laboratory experiments have been performed by Weber [3;4]. During the appraisal of the results it should not be forgotten that the size of the simulated cubes was small compared to the ones experimentally tested. This may cause a difference between experimental and calculated results. While adiabatical simulations are not affected by the size of the concrete spheres the simulations with an open side are. Thus the results should be seen as a first approximation in order to show the general tendencies. The size of the models was limited by the number of elements with whom DuCOM can compute.

Hydration

Weber has shown that the hydration degree after 180 days reached 0.67 and after 360 days 0.82 [3]. The used mixture was comparable to the HB 15. The temperature faltered during the experiments between 15 and 25°C and the humidity between 40 and 50%. This boundary condition was comparable to the situation "2 open sides". After 360 days the calculated hydration degrees of the mixture HB 15 were ranging between 0.76 for 2 open sides, 0.75 for 1 open side and 0.84 for the adiabatical system. For the mixture HB 0 the measured hydration degree was 0.67 after 360 days while the calculated value was 0.73. The difference may be explained by the size effect or simply by the higher humidity during the calculation. Nevertheless the model provides a good estimation for the hydration degree for concretes with light weight aggregates.

Strength development

The compressive strength development is following the curve development of the hydration degree. Table 3 shows the calculated 28 days strength.

Table 3: compressive strength [N/mm^2] after 28 days

t = 28,0 d	fraction of light weight aggregates [%]			
cube	0	15	25	30
adiabatical	139.17	144.59	144.48	144.62
1 open side	57.83	82.70	83.31	105.21
2 open sides	56.66	73.25	72.81	100.73

Laboratory experiments [3] have been performed with the mixture HB 15. The 365 days experimental results are presented in table 4 and compared with the computed ones.

Table 4: Results after 365 days

	experimentally determined compressive strength [N/mm^2]	calculated compressive strength [N/mm^2]
adiabatical	122	144.5
1 open side	120	128
2 open sides	122	125

On the one hand the results for the calculations with one or two open sides seem to be accurate, on the other the value for the adiabatical calculation is overestimated. The experiments performed found that the concrete matrix is dense enough to circumvent any moisture transport from the outside. The simulation did not reproduce this situation exactly. The porosity was during all time steps high enough to simulate a water loss/gain by evaporation/condensation. The adiabatical simulation nearly reached the maximum compressive strength of 145.5 N/mm^2. Hence it can be assumed that the amount of available water was sufficient for complete hydration. So the size-effect, the water loss by evaporation and the fact that the maximum compressive strength was reached are reasons why it can be concluded that the strength development is overestimated but it is accurate enough to provide a first approximation.

Dispersion of moisture

The mixture HB 15 had 150 kg/m^3 water content and additionally 47 kg/m^3 were provided by the saturated aggregates. After 360 days the cube with 2 open sides contained 155 kg/m^3 and the adiabatically stored cube had 175 kg/m^3 water content. The water was found partly chemically bound and partly as liquid in the pores. The calculated results are slightly different. The adiabatical system reached a water content of 170 to 180 kg/m^3 and the cube with an exchange with the environment reached 180 to 190 kg/m^3 The higher water content of the simulated cube with an exchange with the environment can be explained by the higher humidity during the simulation, compared with the experimental conditions.

6. SUMMARY

The modified Chaube model proves to be able to simulate high performance concrete. Some of the results seem to be in compliance with the found laboratory results. Although the experimentally obtained amount of data was very humble and the sizes of the models were smaller than the cubes used for the performed experiments, it can be summarized that:

- the 360 days computed hydration degrees were close to the measured ones. Even though due to the lack of data it was only possible to compare concrete at the age of 180 days and 360 days.

- it was found that the porosity and the early age compressive strength is slightly overestimated by DuCOM. The results for the cubes with an exchange with the environment have been very good. The accuracy of the adibatical simulations have been less reliable.

- the influence of the additionally provided water is measurable. The amount of physically and chemically bound water is corresponding with experimentally found numbers.

- the future development of this model where the water saturated light weight aggregates will be part of the governing equations will improve the accuracy of calculated material parameters.

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