MODELLING OF CONCRETE HYDRATION

MODELLIERUNG DER BETON HYDRATATION

MODELISATION DE L'HYDRATATION DU BETON

Sven Mönnig

SUMMARY

DuCOM is a finite element program which can show the hydration of concrete with any concrete mixtures, to any given time step and different environmental conditions. Comparing calculated temperature distribution, hydration and heat growth rates with measurements a high accuracy was proven.

ZUSAMMENFASSUNG

DuCOM ist ein FEM-Programm, welches die Hydratation von Beton mit beliebigen Betonmischungen, zu beliebigen Zeitschritten und verschiedenen Umgebungsbedingungen darstellen kann. Bei dem Vergleich von errechneten Temperaturverläufen, Hydratationskurven und Wärmezuwachsraten mit gemessenen Laborwerten, zeigt sich eine hohe Genauigkeit von DuCOM.

RÉSUMÉ

DuCOM est un programme d'éléments finis capable de décrire l'hydratation de bétons de compositions arbitraires, à des intervalles arbitraires et pour différentes conditions d'environnement. La comparaison des gradients de température, des courbes d'hydratation et des taux de chaleur calculés avec les valeurs mesurées en laboratoire indiquent une précision élevée de DuCOM.

KEYWORDS: DuCOM, heat growth rate, concrete hydration

1. INTRODUCTION

DuCOM [1] is a program working with concrete finite elements. It is able to deliver a linear description of the hydration of concrete. It provides solutions for pore pressure and temperature at each node of each element for given time steps and environmental condition, i.e. relative humidity and temperature.

Results of porosity, the degree of hydration for every clinker, shrinkage and strength are obtained, too. By implementing DuCOM, a program developed by the University of Tokyo, into MASA [2] the simulation of the influence of hydration on the bearing capacity is possible. To estimate the computational accuracy of DuCOM extended calculations were compared with publications of test results.

2. THEORETICAL PRINCIPALS OF DUCOM

Physical processes like humidity and vapour transport, the hydration of concrete and the development of pore structure are integrated over the volume of a standard reference element. The transport behaviour is simulated on a macro scale. Hydration is simulated by a multi component system which includes the heat development and the amount of available water. The heat development is dependent on the amount of free water. Size and structure of the pores are dependent on the degree of hydration. The pore structure influences the transport behaviour inside the concrete. All the single processes are dynamically linked and dependent on each other as figure 1 should point up.

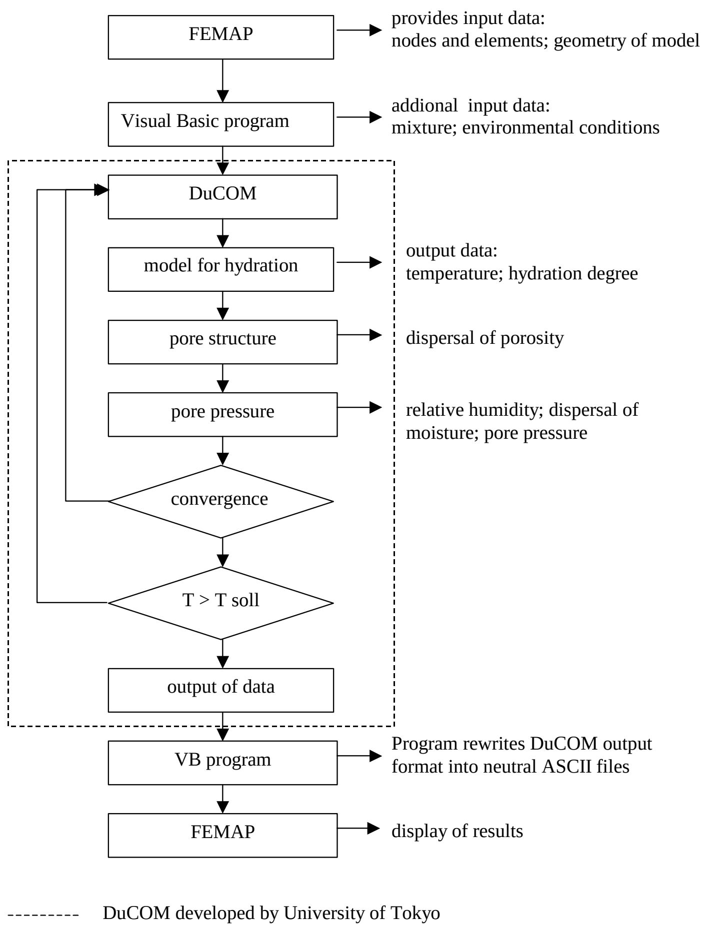

Figure 1: application flow

For further information it is recommended to read “Modelling of concrete performance” [1].

3. LIMITATIONS OF DUCOM

There are some constrictions of DuCOM that should be mentioned. The pore structure is simulated by a consistent distribution of average sized grains. The size is dependent on the amount of cement, fly ash and blast furnace slag. The distance between the grains is based on Blaine values and the size of the grains. Pores are considered to be cylindrically shaped. For the calculation of the hydration the gel and capillary pores are treated as one type.

The assumptions for the moisture transport are non deformable and isothermal material behaviour. Furthermore it is assumed that the total mass of vapour can be neglected compared to the total amount of water. Gas pressure within the material is constant and equals the air pressure. Liquid transport is performed with constant velocity. Thermal effects are negligibly small. These assumptions are based on a representative volumetrically element. All calculations refer to this element.

4. IMPLEMENTATION OF DUCOM

With FEMAP as input and output program it is possible to use a common used program for the visualization of the models. The output file from FEMAP is written in an ASCII format which is translated into the input file for DuCOM. For this transformation a Visual Basic (VB) program was developed by the IWB. While translating the file, the program asks for additional input data. Necessary input information are the time period of the analysis, mixture, Blaine values, temperature of the concrete mixture, temperature and relative humidity of the environment. After the end of the calculation another VB program will translate the result files of DuCOM into an ASCII format which can be read by FEMAP. The results can be graphically presented and furthermore they can be read from MASA and used for continuous analysis of the structure.

5. RESULTS OF SIMULATIONS AND COMPARISON WITH TEST RESULTS

All calculations were based on a 20×20×20 cm^3 cube. The resulting values of the curves were taken at nodes arranged along a line by the centre of a cube.

OPC was simulated with these fractions of clinker:

C_3S	47,2 %
C_2S	27,0 %
C_3A	10,4 %
$C_4(A,F)$	9,4 %

The model of the concrete cube has been scaled by the input program to the size desired by the user. Figure 2 shows the cube before scaling.

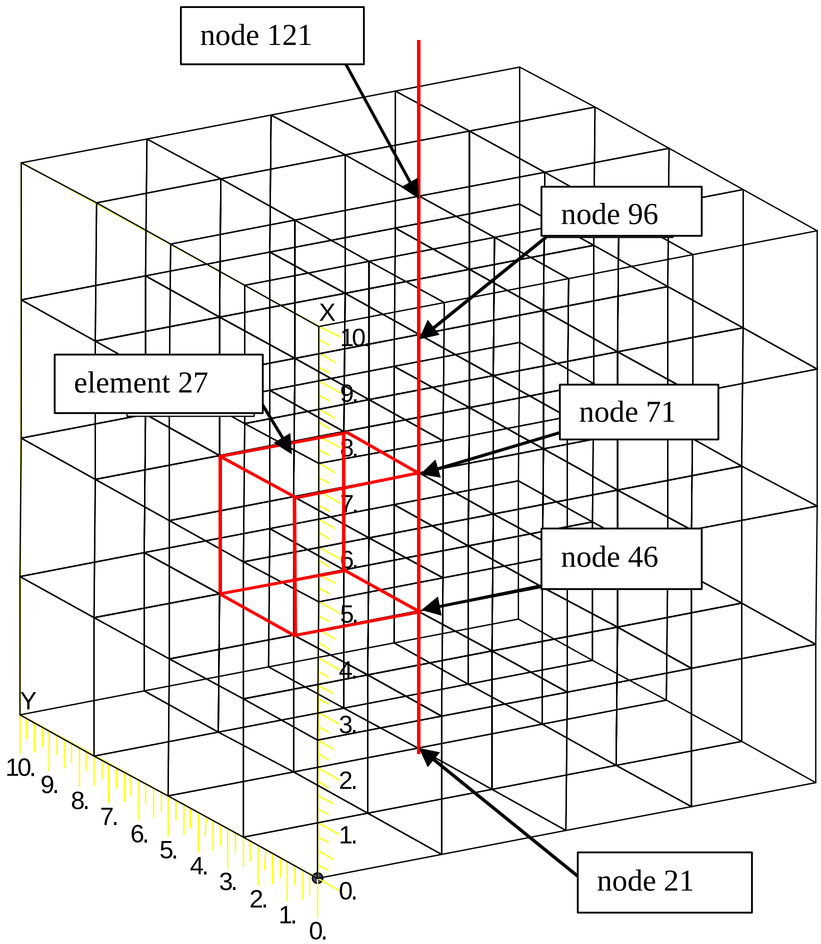

Figure 2: Model of a 20×20×20 cm³ cube

Temperature distribution in a cube

Of interest was the influence of the environment on the development of heat inside the cube. Simulations with an adiabatic system have been performed as well as calculations with one, two, three, four and five sides opened to the environment. The mix temperature was 20°C. The environmental conditions have been assumed constant with 15°C and 100% relative humidity. The concrete mix contained 375 kg/m^3 cement and 1885 kg/m^3 aggregates.

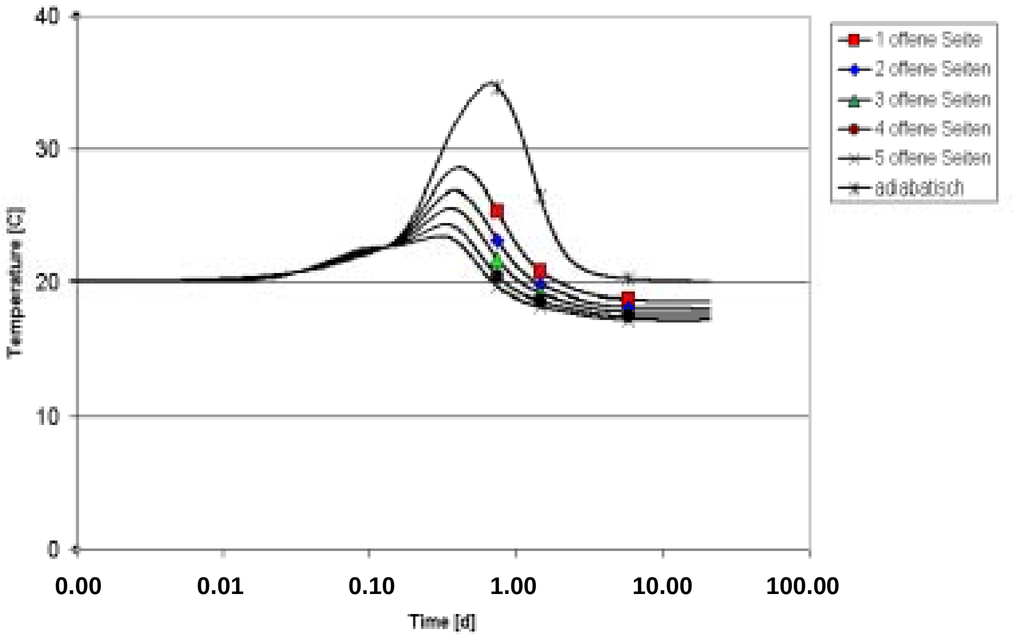

Figure 3: Temperature distribution inside a cube

Degree of Hydration in dependence on the water/cement ratio

The proportion has been changed to a mixture with very high cement content. It contained 836.3 kg/m^3 cement and 1032 kg/m^3 aggregates. These fractions have been chosen to minimize the influence of the aggregates on the water diffusion and the hydration. The reference mixture had a water/cement ratio of 0.4 but the same cement and aggregate content as the others. This mixture has been calculated with five sides open to the environment which had a constant temperature of 15°C and a relative humidity of 100 %.

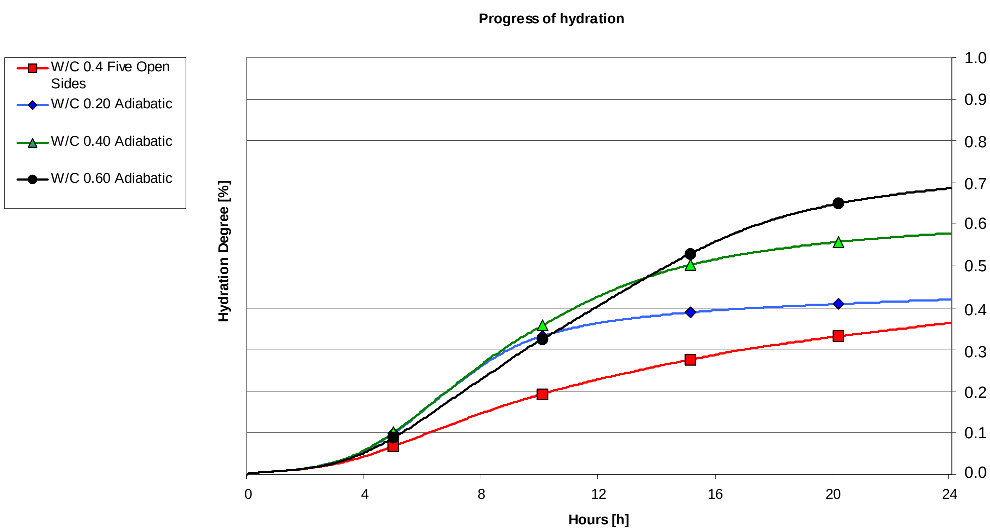

Figure 4: Degree of hydration in dependence on the water/cement ratio

Heat growth rate of clinker

DuCOM provides the overall generated heat for each clinker at each time step. By subtracting the accumulated heat at one time step from the previous one it was possible to calculate the heat growth rate. The curves presented in figure 5 have been interpolated with Excel to abrade them. DuCOM calculated 2500 time steps to reach 24 hours.

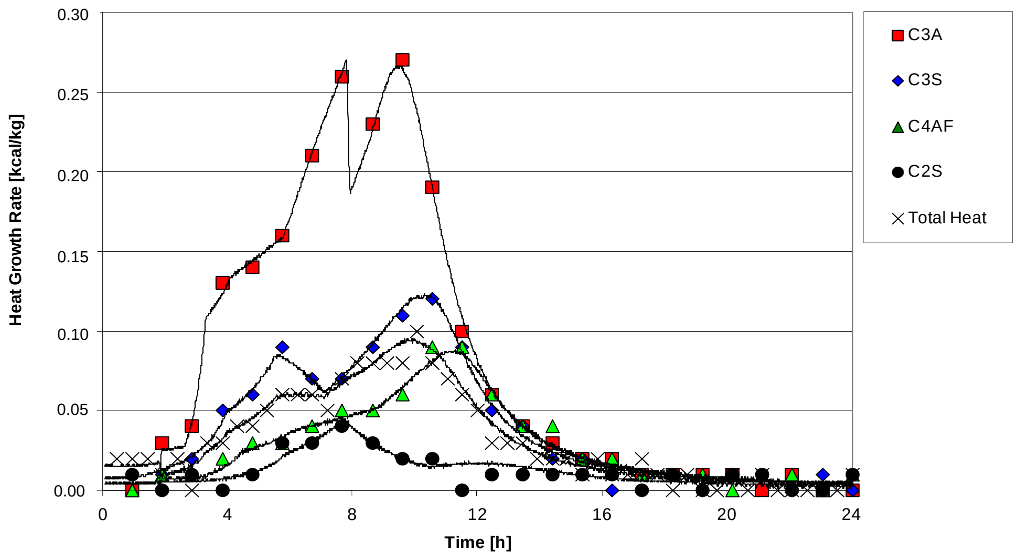

Figure 5: Heat growth rate of clinker

6. DISCUSSION

The maximum temperature of the hydration as shown in figure 3 does reach the extent as expected. Different methods of gaining an approximated value do provide similar results, e.g. the approximation formula for adiabatic heat growth as given in [3] provides likewise results. The results presented in figure 5 follow the expected curves. The influence of the low temperature of the environment on the rate of hydration is reasonable, too. The curves in figure 5 show the same behaviour of the clinker as it was expected due to the specific enthalpy of each clinker.

7. SUMMARY OF RESULTS

DuCOM proved to be very reliable being used for the simulation of hydration of ordinary Portland cements and their mixtures. Temperature development and hydration degree are corresponding with measured values given in the literature. More calculations and experiments should be performed to estimate the accuracy of calculated strength and shrinkage.

REFERENCES

[1] Maekawa, K.; Chaube R., Kishi, T.: *Modelling of concrete performance,* E&FN Spon, London, 1999

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[3] *Zement Taschenbuch 2000*, Verlag Bau+Technik, Düsseldorf, 2000