

# Concrete setting: computer simulation vs. reality

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## I. INTRODUCTION

Computer simulations have become a powerful tool in many fields such as weather forecasting, car crash modelling and flight simulations. Moreover, they can be very useful in the cement research, particularly to model the microstructure development which is difficult to investigate with traditional laboratory equipment at early age.

In this research project, concrete setting, which is the transformation from a suspension to a solid material, is monitored by ultrasonic wave transmission measurements. To relate these measurements to the microstructure development of the cement paste, computer simulations were performed.

## II. SIMULATION SOFTWARE

One of the most commonly used cement hydration models is CEMHYD3D, developed by Bentz [1]. The cement particles are represented by a collection of 3D-pixels (Fig. 1). According to the cement composition, a clinker mineral is assigned to each pixel of these cement particles.

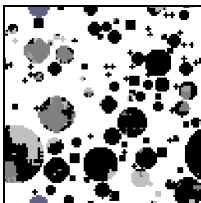


Figure 1. Each grey level in this virtual cement paste represents a particular mineral.

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The chemical reactions between these pixels are simulated by cellular automata algorithms in which the state of a pixel in the next time step is determined by the present state of this pixel and its neighbours.

## III. MATERIALS AND METHODS

The experiments were performed on concrete mixtures with ordinary Portland cement (OPC) as reference and on mixtures in which respectively 30, 50, 70 and 85% of the cement was replaced by blast-furnace slag (BFS). The latter is a by-product of the steel industry with latent-hydraulic properties and is commonly used as a cement replacing additive. The water-to-binder ratio of the mixtures was 0.5.

Ultrasonic measurements were performed with the FreshCon (Fig. 2). With this system velocity, energy and frequency content of ultrasonic pulses sent through the hardening concrete are measured. Initial and final setting times were also determined by the penetration resistance test (ASTM C403).

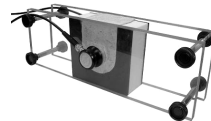


Figure 2. FreshCon container with the attached ultrasonic sensors.

The reaction of cement and water (hydration) is an exothermal process. Besides ultrasonic measurements, the heat release during the hydration of a cement paste sample of the same composition was measured in an isothermal calorimeter at 20°C. In this way, the measured heat release can be compared to the heat release calculated by CEMHYD3D to verify the accuracy of the model.

## IV. RESULTS AND DISCUSSION

### A. Hydration heat

The heat release during the hydration, measured in the calorimeter and simulated by CEMHYD3D corresponds well for the reference mixture (Fig. 3). However, if more than 50% of the OPC is replaced by BFS, CEMHYD3D tends to simulate less heat than actually produced. The influence of the BFS reaction is probably underestimated by the model.

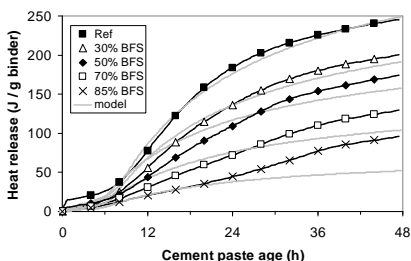


Figure 3. Heat release vs age for mixtures with increasing percentages of OPC replaced by BFS.

### B. Setting

To investigate setting behaviour with CEMHYD3D, the fraction of particles bound together by hydration products can be calculated at different ages (Fig. 4a). Ye [2] compared similar calculations to ultrasonic measurements and found for OPC concrete that the wave velocity started to increase rapidly when the cement hydrates form complete pathways of connected particles. This percolation threshold corresponds to the setting. However, the measured wave velocities (Fig. 4b) start to increase sooner than the solid percolation. This can be attributed to bleeding, internal settling and the formation of hydration products not contributing to the setting. The solid percolation corresponds well to the initial and final setting determined by the standard penetration resistance test (grey dots, Fig. 4a).

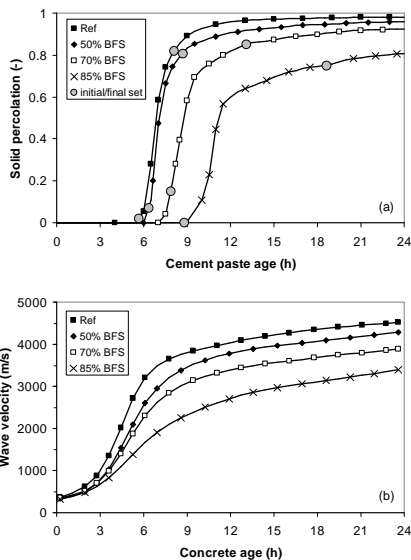


Figure 4. (a) Fraction particles bound together in the cement paste (CEMHYD3D simulation) and (b) ultrasonic velocity measurements

## V. CONCLUSIONS

CEMHYD3D is a useful tool to study the setting of concrete, but the implementation of BFS can still be approved. The relation between the ultrasonic measurements and the percolated solid fraction as simulated by CEMHYD3D will be investigated more thoroughly.

## ACKNOWLEDGEMENTS

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## REFERENCES

- [1] D. Bentz, *Modelling cement microstructure: Pixels, particles and property prediction*, Mater Struct, 32, 187-195, 1999.
- [2] G. Ye, *Experimental study and numerical simulation of the development of the microstructure of cementitious materials*, PhD thesis, TU Delft, 2003.