Print Go Back Next Page

Computer 3D Microstructure Modeling And Prediction Of Hydration And Strength Of Lunar-like Cement With Steam

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Summary: This paper presents an attempt to create a computer based cement hydration model for three types of cements, one conventional and two lunar type cements. Here, lunar cements are named like that as their compounds are very similar to the candidate lunar materials.Using such simulants is efficient in order to simulate and predict lunar cement properties and behavior. Computer simulation is based on that developed by NIST 3D hydration and microstructural model. Four different models are established for the lunar and portland cements. Models represent two wet mixtures with lunar cement, one is with addition of gypsum and both lunar cement and conventional portland cement threaten under dry-mix / steam injection (DMSI) method. In order to simulate the dry-mix / steam injection hydration process, the algorithm in the 3D computer simulation program is modified respectively with the different nature of steam hydration, hydrates formed, their amount and formation in time line. Based on the derived simulation models, the hydration process, morphological and chemical compositions of the hydrates formed, percolation properties of the different mixes are compared. An evaluation of the predicted properties and experimentally determined is carried out as well. The results show that this type of computer modeling and behavior prediction could be very useful in order to plan and evaluate costly and unique (like in case with lunar cement) experiments.

Keywords: Microstructure modeling; hydration; strenght development; computer image-based model; percolation.

1 INTRODUCTION

In the present studies on materials which could be produced in outer space and the moon, concrete is considered as one of the suitable materials. There are studies regarding possibilities to produce cements from lunar materials and materials which chemical compounds are very closed to lunar one (Horiguchi et al. 1996). Actually many constrains exist if the experiments with real lunar materials are to be conducted. Main are the availability of the real lunar materials and if substitutes are used, how close to the real one they are. It will be very helpful if computer-based models of microstructure of such cements, hydration process and transport properties could be created and used (Bentz 1997).

The major work in computational materials science of cement and concrete and computer-based models dates from the last 10 to 15 years and is powered by the advancements and progress made in the computer processing speed and memory capacity. Cement and concrete as a random materials are a very suitable object to be characterized, described and predicted in its properties by applying computer-based models. Such models are developed for describing interfacial transition zone (ITZ), microstructure in concrete; leaching of (calcium hydrates) CH from microstructure; set point determination; hydration rates, heat of hydration, and chemical shrinkage; effects of cement particle size distribution (PSD) on cement and concrete properties (Bentz 2000). The development and use of similar computer image-based models will highlight the microstructure characteristics of lunar like (high aluminates) cements.

Another important point to consider is that dry mix/steam injection method is belived to be applicable for moon or outer space environment. But the hydration process develops in this type of system diferently. It is important to create a computer based model for the hydration and microstructure in dry mixes subjected to steam injection.

2 OBJECTIVE

The objectives of this study are: to reconstruct 3D digital microstructure of two high aluminate cements, one of them with a gypsum addition and one ordinary portland cement, which are tested in two ways: conventional (wet mixtures) and DMSI (dry mixtures); to estimate the hydration rate and compressive strength based on the established models; to compare predicted results with the measured one from previous experiments.

3 BACKGROUND

Both the computer image based models and dry mix/steam injection method are relatively new technologies which developments aim to highlight the microstructure of existing and future materials with enhanced behaviour. The results of previous studies (Lin et al. 1998) showed that DMSI causes rapid hydration and very high strength compare to wet mix method, which is a strong base for further research.

4 COMPUTER IMAGE-BASED MODEL

4.1 Testing Procedure

Here, experimental data from two different sources have been used (Horiguchi et al. 1996; Lin et al. 2000) in order to construct computer image-based model representing the microstructure before and after hydration. The details for the mixtures used are given in the Table 1 below:

Table 1. Mixtures names, cement fineness and types, curing conditions and compressive strength.

Type Cement	Mixture	Fineness m^2/kg	W / C	Curing	SEM Image	CS –24h (MPa)	CS –3/7 d. (MPa)
Lunar	WM1	357	0.835	Wet	CD357	N.A.	8.4/12.2
Lunar+Gyp	WM2	357	0.600	Wet	CD357	N.A.	1.9/2.9
Lunar	DMS	357	0.2	Dry	CD357	21.9	N.A.
Port	DMO	387	0.2	Dry	CU387	38.8	N.A.

According to the reference source (Horiguchi et al. 1996), for all different cements, a series of 4 cm mortar cubes were prepared. The standard Japanese mix procedure is applied where the weighed cement, sand and water (as shown in Table 2) were mixed in a electric powered mixer for 4 minutes. The fresh mortar then was cast in 4x4x16 cm prismatic molds. After compacting and finishing, the mortar test specimens were cured at 20 degree C and 60% humidity for wet mix method, and into autoclave unit for steam curing at 170 C and pressure of 7 kgf/cm^2 for 24 hours. The temperature regime is presented on Fig. 1.

Table 2. Mix Proportions for Wet Mixes (Horiguchi et al. 1996) and Dry Mixes.

Code	Water, cc	Cement, g	Sand, g	W/C
WM1	334	400	800	0.835
WM2	240	400	800	0.600
DMS	0	400	800	0
DMO	0	400	800	0

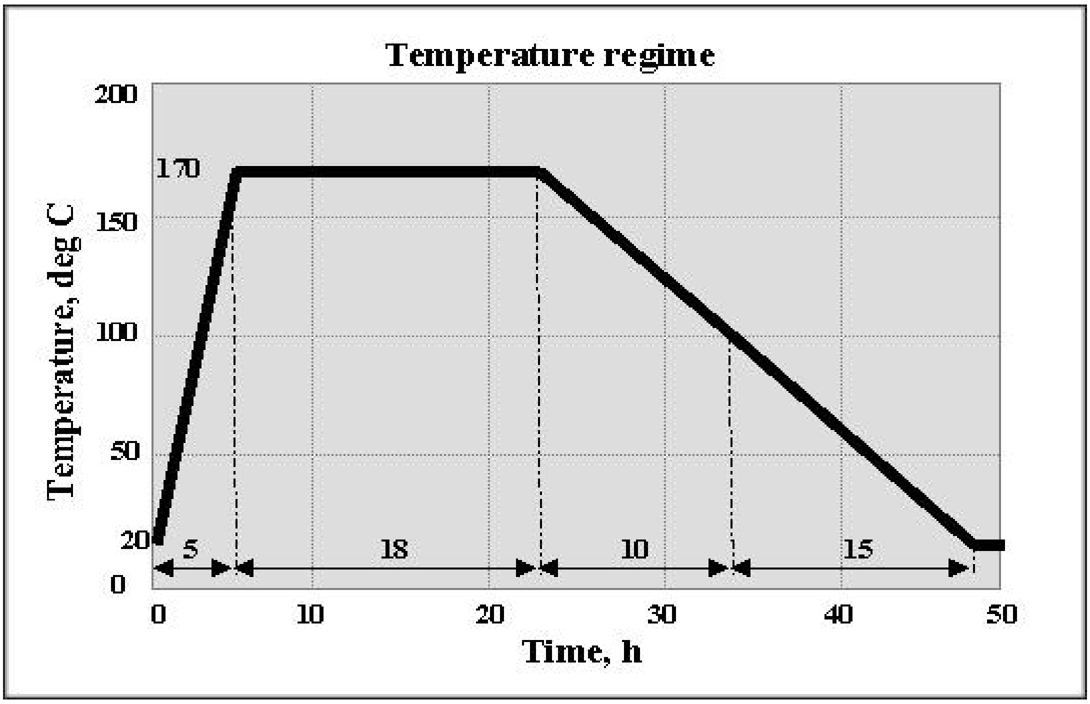


Figure 1. Temperature regimes for dry mix / steam injection.

After the curing, the test specimens were tested to determine the hydration products (by X-ray diffraction) and scanning electronic microscopic analysis for highlighting the morphological features of hydration products. Also examined are the degree of hydration and compressive strength.

4.2 3D Digital reconstruction of microstructure

The reconstruction and 3D microstructure generation and hydration simulation proces'flow diagram is presented on Fig. 2.

4.2.1 Generation of 3D image and distribution of phases

According to the procedure for generation of 3D microstructure of cement and concrete (Bentz 2000), a scanning electron microscope image and particle size distribution are the initial inputs. Particle size distribution is on a number basis, and the phase volume fraction and phase area fraction are obtained based on digital SEM images. Then by applying the developed programs for reconstruction of initial 3D microstructure (Bentz 2000), its first approximation is received. Further, the distribution of phases based on phase volume and phase area fractions is performed by applying NIST procedure. Figure 3(a, b, c, d) presents the data input, images,

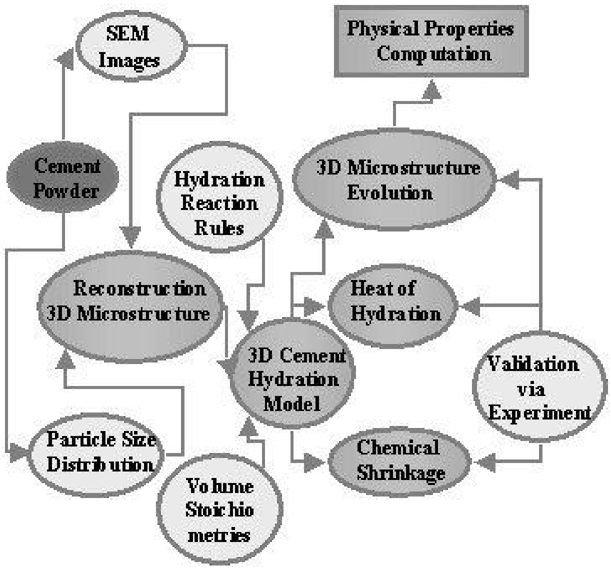
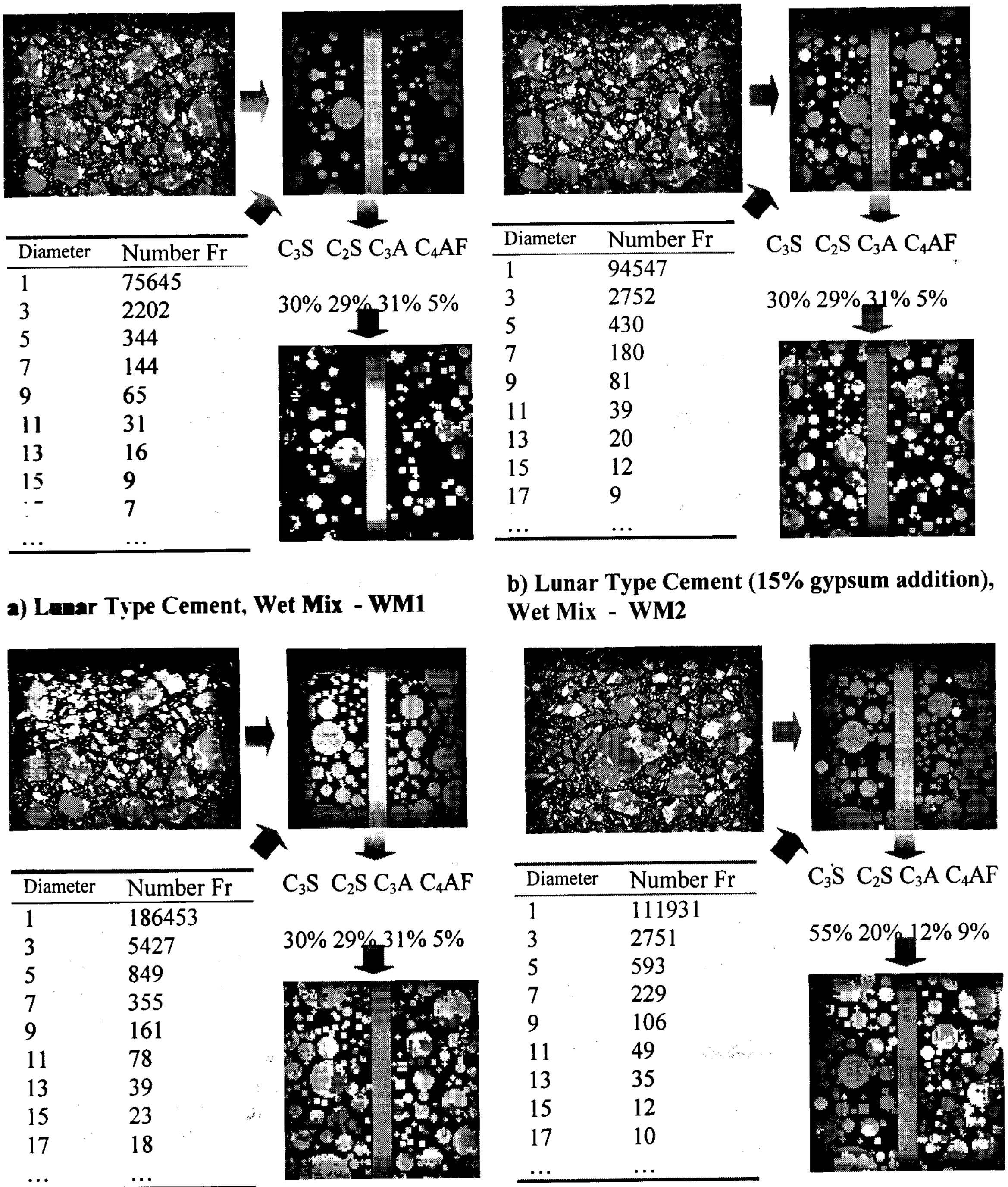


Figure 2. Modeling and experimental flow for hydration simulation.

Go Back Next Page



Diameter	Number Fr
1	75645
3	2202
5	344
7	144
9	65
11	31
13	16
15	9
[illegible]	7
...	...

a) Lunar Type Cement, Wet Mix - WM1

Diameter	Number Fr
1	94547
3	2752
5	430
7	180
9	81
11	39
13	20
15	12
17	9
...	...

b) Lunar Type Cement (15% gypsum addition), Wet Mix - WM2

Diameter	Number Fr
1	186453
3	5427
5	849
7	355
9	161
11	78
13	39
15	23
17	18
...	...

c) Lunar Type Cement, Dry Mix/Steam Injection DMS

Diameter	Number Fr
1	111931
3	2751
5	593
7	229
9	106
11	49
13	35
15	12
17	10
...	...

d) Portland Type Cement, Dry Mix/Steam Injection - DMO

Legend: C_3S C_2S C_3A C_4AF Gypsum Water Porosity Aggregates

Figure 3. SEM Images, PSD, 2D slices of 3D initial digital mono microstructure and the same after the distribution of the phases for the lunar and portland cements and for wet &dry mixtures.

PSD tables and the initial 2D slices of 3D mono C_3S microstructure and all phases'microstructure after the distribution. The assumptions are: the resolution is 1 μm/pixel; particles are placed from largest to smallest; gypsum (volume fraction from the total) and cement follow the same particle size distribution.

4.2.2 Hydration reaction rules

In the present version of a 3D cement hydration and microstructure development modeling package CEMHYD3D (Bentz 2000), the hydration simulation is based on phases, reactions to be considered in the hydration and the rules for the dissolution of solid material, the diffusion of the generated diffusing species, and the reactions of diffusing species with each other and with solid phases. In the reconstructing of the wet mixtures microstructure (WM1 and WM2), the same assumptions for the phases, reactions and the rules in the cellular-automata are applied. But for the reconstruction of dry mixtures some modifications are proposed and applied.

Reactions and rules applied to wet mix cement test specimens. The hydration of wet cement mixtures is well studied by many scientists (Taylor 1990; Mindess and Young 1981) and consists of dormant, acceleration (including setting) and deceleration periods. Through the dormant period not significant changes occur, through the acceleration period most of calcium silicate hydrate (CSH) and calcium hydroxide (CH) gel is formed and in the deceleration period, tricalcium aluminate (C3A) and tetracalcium aluminoferrite (C4AF) are surrounded by CSH and gradually become stronger. The cement model reactions (Bentz 1997) included in NIST model are:

a) Silicate reactions

$C_3S + 5.3H \rightarrow C_{1.7}SH_4 + 1.3CH$ $C_2S + 4.3H \rightarrow C_{1.7}SH_4 + 0.3CH$

b) Aluminate and ferrite reactions

$C_3A + 6H \rightarrow C_3AH_6$ $C_4AF + 3CSH_2 + 30H \rightarrow C_6AS_3H_{32} + CH + FH_3$

$2C_3A + C_6AS_3H_{32} + 4H \rightarrow 3C_4ASH_{12}$ $2C_4AF + C_6AS_3H_3 + 12H \rightarrow 2C_4ASH_{12} + 2CH + 2FH_3$

$C_3A + 3CSH_2 + 26H \rightarrow C_6ASH_{32}$ $C_4AF + 10H \rightarrow C_3AH_6 + CH + FH_3$

These reactions are implemented in cellular automata rules for the dissolution of solid material step, the diffusion of the generated diffusing species step, and the reactions of diffusing species with each other and with solid phases step.

Reactions and rules applied to dry mix/steam injected cement test specimens. The hydration of dry mix/steam injected cement mixtures is not so well studied and analysed and its research continues. Though some studies provide ideas on the reactions and hydration under steam treatment (Horiguchi et al. 1996; Lin et al. 1998; Lin et al. 2000).

According to them, the steam condenses and forms a moist coating on the cement particle surface. The moist coating thickness increases with the increase of steam condense as a result of capillary pressure. As a result the cement compounds along the contact area start to dissolve and later to form calcium silicate hydrate (CSH) gel. Main difference is that the moisture coating is not sufficient to dissolve calcium oxide in the cement compounds in order to form calcium hydroxide (CH) crystals, which are the first to be formed in wet mix cement.

The reactions to be considered then in the model are:

a) Silicate reactions

$2C_3S + 3H \rightarrow C_5S_2H_2 + CH$

$C_2S + 1.17H \rightarrow C_{1.7}SH_{0.87} + 0.3CH$

b) Aluminate and ferrite reactions

$C_3A + 5.56H \rightarrow C_3AH_{5.56}$

$C_4AF + 6.33H \rightarrow C_{3.4}(A,F)H_{5.73} + 0.6CH$

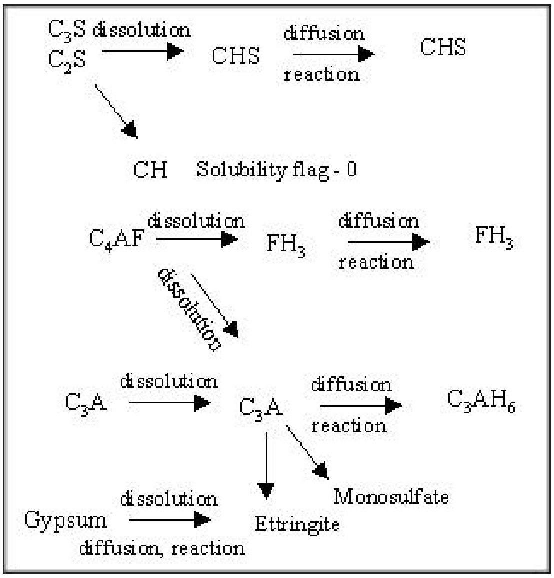


Figure 4. Dissolution, diffusion and reaction scheme.

Then the proposed modified scheme for the dissolution, diffusion and reaction steps is seen

In Fig. 4. Compared to the model presently included in NIST, here the calcium hydroxide is consider initially to be not soluble, and the solubility flag is 0 for CH pixels. Another difference is that the dissolution, diffusion and reaction of C_3S and C_3A occur with accelerate speed as a result of the steam pressure in the very beginning of the hydration process.

5 RESULTS AND DISSCUSION

After execution of the NIST 3D model and the modified one, the 2D slices of 3D hydrated microstructure is presented in Fig. 5, then the hydration degree, compressive strength and percolation of solids versus hydration are estimated and plotted on Fig. 6 and Fig.7. While simulating the steam hydration the defined temperature regime is applied (described in Fig.1), and the activation energy is converted to the one, which corresponds to the curing conditions. The solubility flag of CH pixels is set to 0 as well.

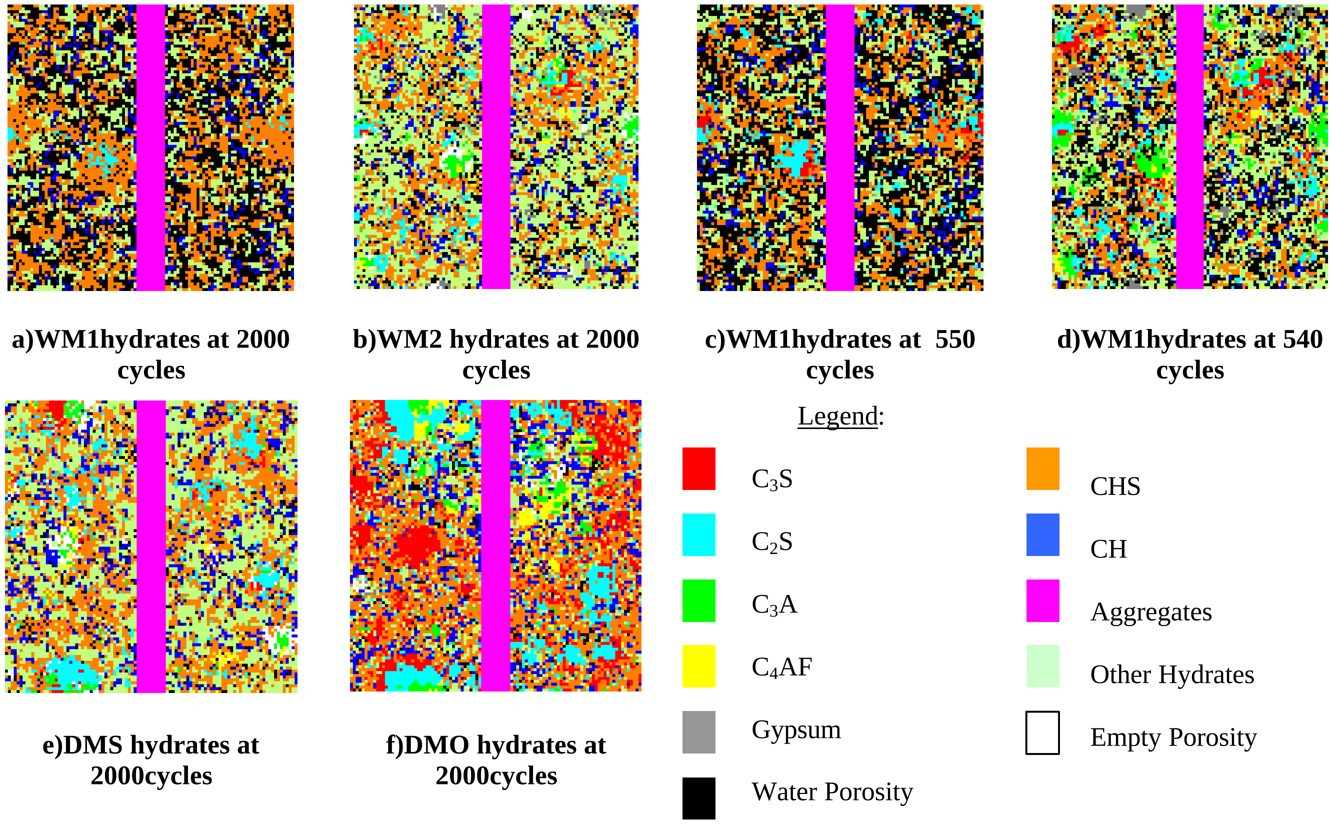


Figure 5. 2D slices of 3D hydrated microstructures.

The results on Fig.5 give an idea for how the microstructure has changed with the cycles elapsed from the start of the hydration. As the WM1 mixture is with very high W / C, the water porosity is still present and not reach by solid phases even at 2000 hydration cycles. The WM2 mixture shows different hydration development, as a result both of W / C and presence of gypsum, which continues to react with C_3A until is entirely consumed. The hydration occurs faster than in case of WM1 mixture and at 2000 cycles already an empty porosity is observed. On the other hand, steam injected and dry mixtures as a result of almost zero W / C show very intensive hydration in the early stage, proved by the graphics on the right side of Fig.6. The 2D slices of the 2000 cycles hydrated DMS and DMO microstructures also show the distribution of hydrated products, and an empty porosity in DMS case can be observed. It could be explained with the fact that CH is formed in less amount than compare to wet mixtures.

When compare the compressive strength of both predicted (based on the model) and experimentally measured (Table 1), good agreement is found in case of WM1 and DMO mixtures but significant discrepancy in case of WM2 mixture and slight in DMS case. Two reasons could be indicated: the high volume presence of gypsum in WM2 mixture, and the approximate SEM input images used.

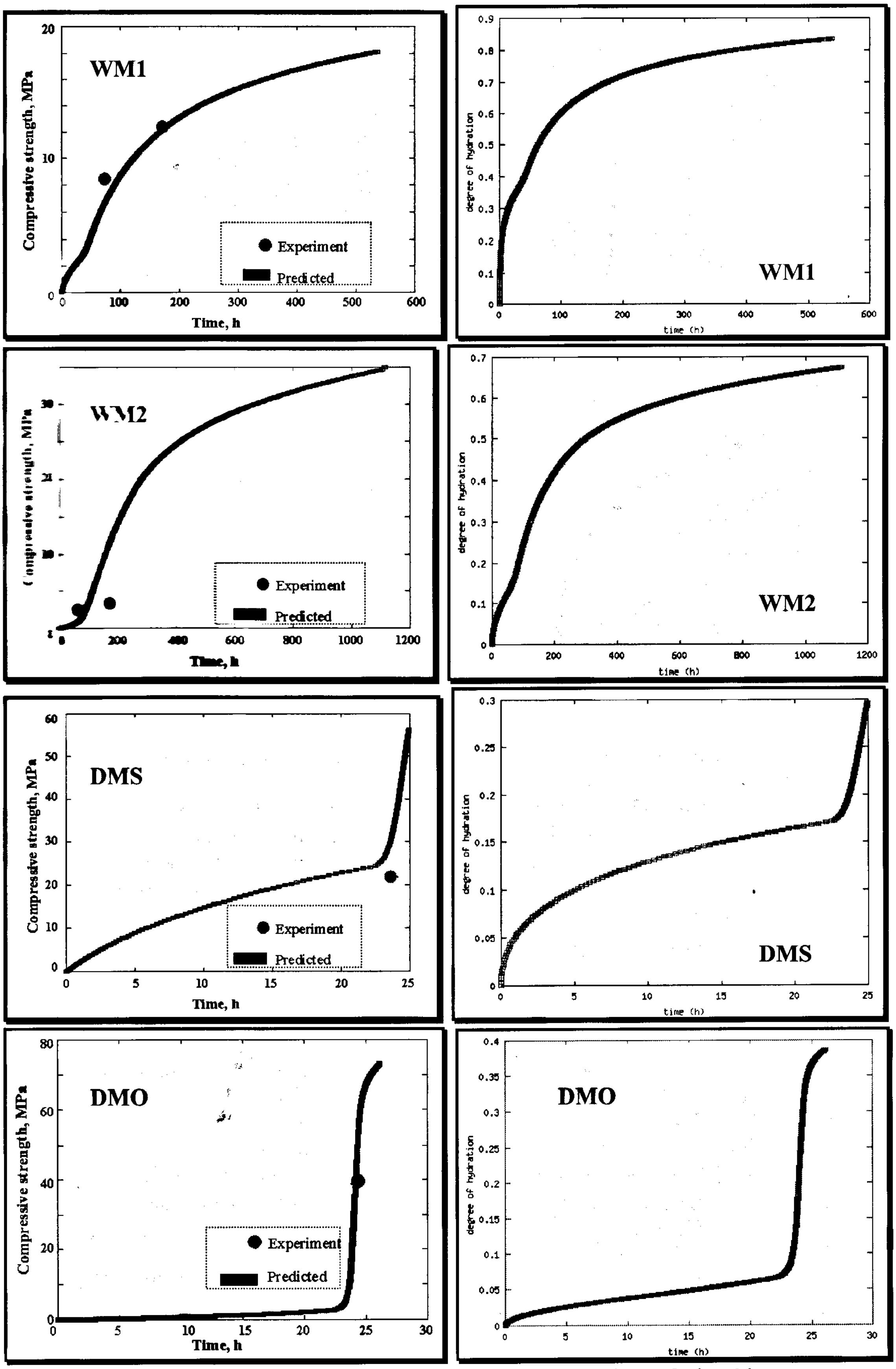


Figure 6. Compressive strength-time and hydration-time relationships.

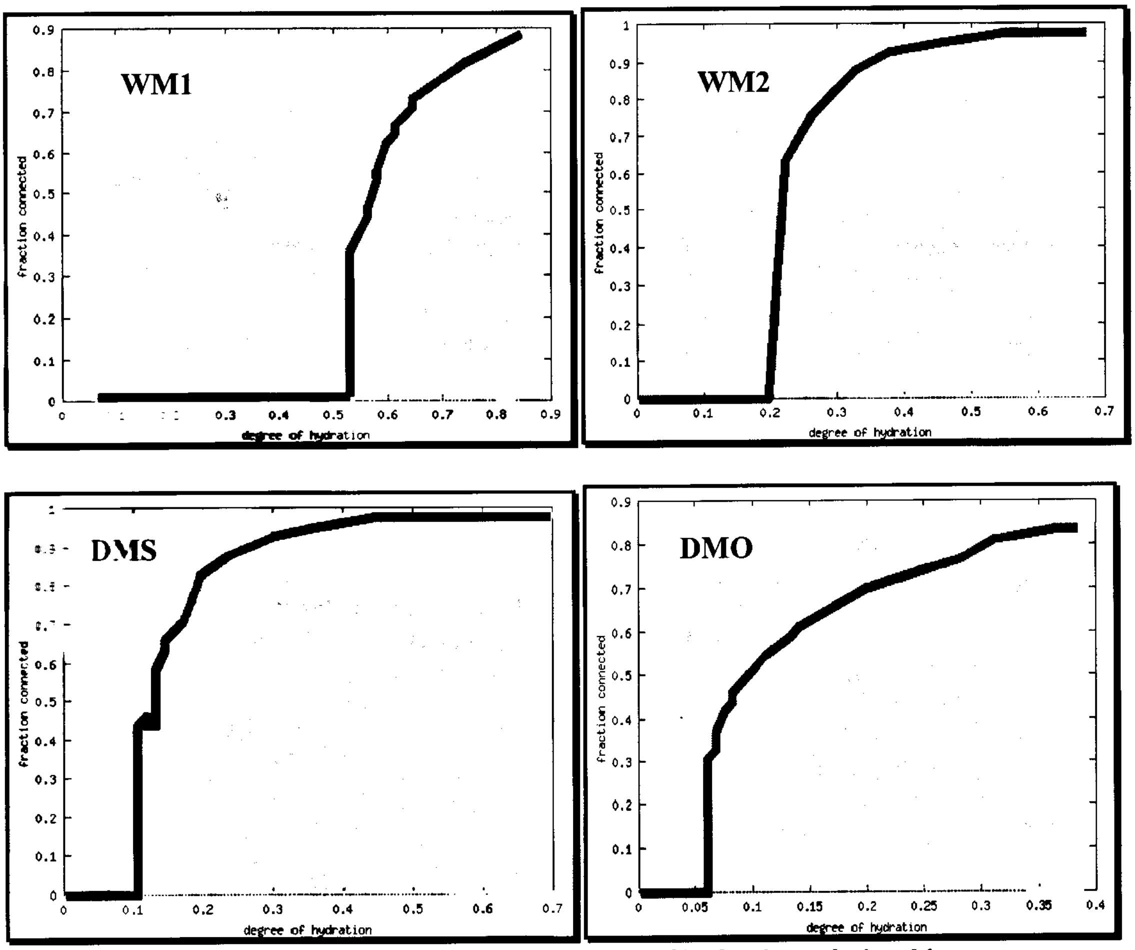


Figure 7. Percolation of solids – degree of hydration relationship.

The solid percolation and degree of hydration relationships for the four studied cases reveal that hydrates are formed on quite early stage when steam injection is applied. In case of large W / C (WM1) fractions get connected only at 0.5 hydration degree, and with the decrease of W / C – much earlier: 0.2 hydration degree in case of WM2, and about 0.1 in DMS/DMO case.

6 CONCLUSIONS

Based on the simulation, the models established, and the comparison with some experimental results, it could be summarized that computer image based models are good tool to predict physical and transport behaviour of cements and concrete. The simulation results show that W / is significant factor for developing of hydration. Predicted and experimentally measured compressive strengths showed relatively good agreement with exception of the case of WM2 mixture. It is of great importance to have an accurate characterization of the starting materials in order to develop a realistic hydration model. It is necessary to conduct more experimental tests and simultaneously develop realistic describing them models.

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8 REFERENCES

1. Bentz, D. 1997, ‘Three-dimensional computer simulation of portland cement hydration and microstructure development’, in Journal of American Ceramic Society, 80 [1], pp. 3-21.

2. Bentz, D. 2000, *CEMHYD3D: A Three-Dimensional Cement Hydration and Microstructure Development Modeling Package. Version 2.0*, Building and Fire Research Laboratory, National Institute of Standards and Technology, NISTIR 6485, April.

3. Horiguchi, T., Saeki, N., Yoneda, T., Hoshi, T. & Lin, T. 1996, ‘Study on lunar cement production using Hokkaido Anorthite and Hokkaido space development activities’, Proc. 5th Int. Conf. on Space’96, Albuquerque, NM, USA, 1-6 June, Vol.1, pp.621-629.
4. Lin, W., Lin, T., Hwang. C. & Peng, Y. 1998, ‘Fundamental study on hydration of cement and cement minerals with steam”, in ACI Materials Journal, V.95, No1, January-February, pp.37-49.
5. Lin, W., Hwang. C. & Peng, Y. 1998, ‘Characteristics of microhydrates formed under steam conditions’, in ACI Materials Journal, V.97, No3, May-June, pp.309-324.
6. Mindness, S. & Young, J.F., 1981, *Concrete*, Prentice-Hall, Inc., New Jersey.
7. Taylor, H.F.W., 1990, *Cement Chemistry*, Academic Press Limited, London