# Materials Science and Intelligent Technologies Applications

Edited by
Khanittha Wongseedakaew and Qi Luo

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# Materials Science and Intelligent Technologies Applications

Selected, peer reviewed papers from the
2014 3rd International Conference on
Key Engineering Materials and Computer Science
(KEMCS 2014),
August 5-6, 2014, Singapore



*Edited by*

**Khanittha Wongseedakaew and Qi Luo**

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# Preface

2014 3rd International Conference on Key Engineering Materials and Computer Science (KEMCS 2014) will be held on August 5-6, 2014, Singapore. KEMCS 2014 is an integrated conference concentrating its focus upon Key Engineering Materials and Computer Science. The conference promises to be both stimulating and informative with a wonderful array of keynote and invited speakers Prof. Gerald Schaefer from Loughborough University, UK

Materials science is an interdisciplinary field applying the properties of matter to various areas of science and engineering. This scientific field investigates the relationship between the structure of materials at atomic or molecular scales and their macroscopic properties. It incorporates elements of applied physics and chemistry. With significant media attention focused on Nanoscience and nanotechnology in recent years, materials science has been propelled to the forefront at many universities. It is also an important part of forensic engineering and failure analysis. Materials science also deals with fundamental properties and characteristics of materials.

In order to meet high standard of "Advanced Material Research, the Organization committee has made their efforts to do the following things,

Firstly, we start to call for papers in January 10, 2014. During the past 4 months, we have been received 380 papers, but poor quality paper has been refused after reviewing by anonymous referee experts.

Secondly, all the papers have gone through a peer-review process for their originality and quality. The topics covered in this book include:

Chapter 1: Materials Science and Materials Engineering
Chapter 2: Artificial Intelligence and Data Mining, Data, Image and Signal Processing, Intelligent Automation and Control
Chapter 3: Computer Science and Information Technologies
Chapter 4: Electrical and Magneto electric Applications
Chapter 5: Advanced Technologies in Social, Education, Economics, Statistics and Management Applications

In the proceeding, you can learn much more knowledge about Key Engineering Materials and Computer Science of researchers all around the world.

I am thankful to colleagues for their contributions to KEMCS 2014. I should also like to thank the members of the Organizing Committee and the corporate sponsors for their efforts and contributions towards making the conference a success. Special thanks go to TTP Publisher Our sincerely acknowledgements are also expressed to the people who contribute to the proceedings and conference. Moreover, my thanks are also due to the sponsors for providing much help for the conference.

Finally, I hope the attendees benefit from the conference, and have a happy and meaningful journey in Singapore.

Khanittha Wongseedakaew and Qi Luo

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# CHAPTER 1:

# Materials Science and Materials Engineering

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# Modifications in Water Sorption Isotherms of Cement Mortars Caused by Carbonation: Effects of Cycles

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**Keywords:** Water adsorption; Carbonation; Pore size distribution; Humidification drying cycles

**Abstract.** This work aimed to examine the influence of carbonation on the water sorption isotherms of cement materials. Two types of normalized CEM I and CEM II Portland cement mortars were carbonated at 20°C, 65% relative humidity and 20% of $CO_2$ concentration for 32 days. The pore size distributions determined from the water sorption showed a reduction in microporosity and a slight increase in the mesoporosity. The pores clogging due to formation of calcium carbonate was highlighted by the reduction of the quantity of adsorbed water and the decrease in the hysteresis isotherms. We also studied the coupling effect between carbonation and humidification-drying cycles. The results of this study also indicated that the humidification-drying cycles coincide only from the second cycle because of a difficult evacuation of water during desorption, even at low humidity.

## Introduction

Carbon dioxide from the air can react with the portlandite $Ca(OH)_2$ and the calcium silicate hydrate C-S-H in concrete to form calcium carbonate $CaCO_3$. This process is called carbonation, which is a natural aging process for all cement materials. This transformation is accompanied by a decrease in pH. The principle reactions are:

$$CO_2 + Ca(OH)_2 \rightarrow CaCO_3 + H_2O \quad (1)$$

$$C_xS_yH_z + xH_2CO_3 \rightarrow xCaCO_3 + ySiO_2.tH_2O + (x\text{-}t+z)\,H_2O \quad (2)$$

The progress of these carbonation reactions causes modifications in the microstructure, which is highlighted by various parameters such as variations in water content. The carbonation reactions of portlandite and C-S-H indicate that the process releases part of the water of hydrate structures. Therefore, the carbonation at first induces a local accumulation of moisture in the pores. Pihlajavaara [1] observed an increase in the quantity of evaporable water content in carbonated materials by drying at 105°C. This released water can certainly participate in the composition of the interstitial solution and contribute to the transport of corrosive agents.

This excess water will be evacuated after a certain time and the material will be in equilibrium with environmental moisture. Houst [2] and Johannesson and Utgenannt [3] observed that, at a given relative humidity, the carbonated mortar contains less water than the non-carbonated one. This decrease in water content is probably due to the reduction in porosity as a result of carbonation. Thus, Meyer [4] found that carbonated concretes dried faster than non-carbonated ones.

Some authors present the water activity by the saturation level and they also find that, for a relative humidity equal to 65%, the saturation ratio of non carbonated material is higher than that of the carbonated material, which is coherent with the reduction of porosity after carbonation [5], [6].

However, the concrete structures in-situ is also subjected to humidification-drying cycles, which results in a much more complicated water activity. This has motivated us to perform this work in order to approach the laboratory results to in-situ results. In this work, the water activity of non-carbonated and well-carbonated cement mortars were firstly studied using water vapor adsorption. Then we examined the effects of humidification-drying cycles on the water activity. The pore size

distributions were also calculated from water vapor adsorption desorption isotherms in order to study the micro structural changes caused by carbonation.

## Materials and methods

**Mortar.** The cements used in this study were:

CEM I 52.5 N PM-ES-CP2

CEM II / B-M (LL-V) 32.5 R

These cements were fabricated by Lafarge company in accordance with European norm EN 197-1 "Cement – Part 1: Composition, specifications and conformity criteria for common cements".

The CEM I and CEM II mortars were prepared by mixing respectively the cements CEM I and CEM II with French normalised sand certified in accordance with norm EN 196-1 and ISO 679:2009. The water/cement and sand/cement ratios were 0.5 and 3, respectively. At the end of the mixing, the mortar was placed in cylindrical moulds (Ø = 40 mm, h = 60 mm) and stored in a humid chamber in order to avoid precocious desiccation in the vicinity of the surface exposed to drying. The samples were demoulded after 24 hours and then cured in water for 90 days in a humid chamber (20°C, 100% relative humidity). The cure in water prevents the natural carbonation during storage.

Bier et al. [7] observed the creation of macroporosity after carbonation of a mortar, which was not rich in portlandite and contained fly ash. The CEM II is poor in portlandite in comparison with CEM I, and therefore the CEM II was also chosen for this study because we want to ensure significant changes not only in the micro porosity but also in the domains of meso and macro pores.

**Pre-treatment.** We employed a method of pre-treatment basing on the work of Thierry [8] and Parrot [9]. The specimens are dried at 105°C until constant weight. Finally, the specimens are placed for 7 days in a climatic chamber at 65% relative humidity. The advantages of this method are to homogenise the internal humidity in the samples and to prevent the natural carbonation during the pre-treatment process.

**Carbonation test.** To implement the test, the specimens were subjected to $CO_2$ in an environmentally controlled chamber at 20°C, 65% relative humidity and 20% $CO_2$ concentration for 32 days to ensure a complete carbonation. The carbonation device consists of a climatic chamber Vötsch VP1300 connected to a $CO_2$ tank (Figure 1). The concentration of $CO_2$ in the chamber is controlled by an automatic $CO_2$ regulator.

Samples collected in carbonated and non-carbonated specimens were then grinded into powders to 80 μm using a mortar – pestle and a sieve, and subsequently used for water adsorption.

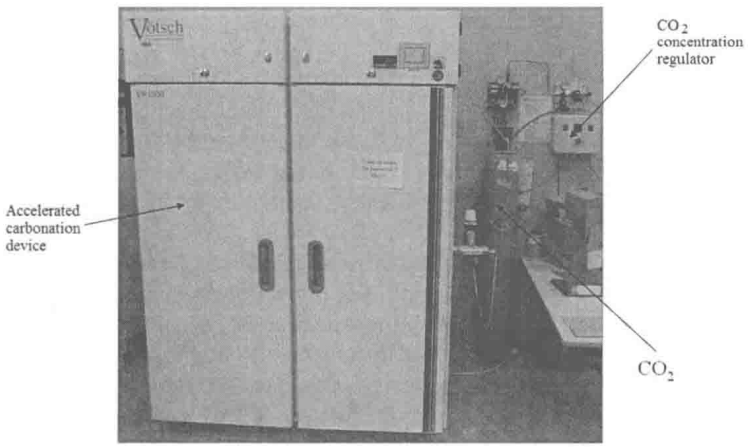


Fig.1 Accelerated carbonation test device

**Water adsorption.** It is well known that cement paste has a multiscale structure that spreads from the nano- and microstructure to the mesoscopic scale and then to the macroscopic scale, which is visible to the naked eye. The nano- and microscopic scales consist of sheets of C-S-H. These sheets associated with packets are called grains and constitute a second level of the observation, which is the mesoscopic scale.

We examined the water vapor adsorption on grinding powders originating from the test samples to study the microscopic scale. For this test, we used a humidification regulator connected to the microbalance of the thermal analysis Mettler Toledo machine (Figure 2). The regulator controlled automatically the temperature at 20°C and changed the relative humidity every one hour.

The sorption steps are: 5%-10%-20%-30%-40%-50%-60%-70%-80%-90%-95%.

The desorption steps are : 95%-90%-80%-70%-60%-50%-40%-30%-20%-10%.

Change in mass of the sample was automatically followed by the microbalance (Figure 3). This method is also known as the dynamic adsorption.

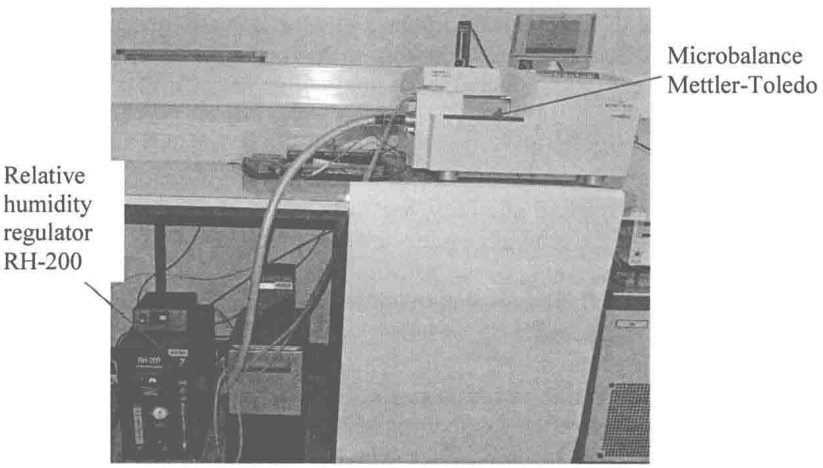


Fig.2 Water sorption device

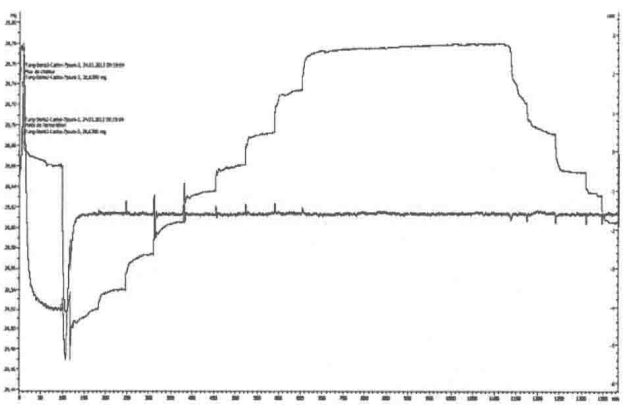

Fig.3 Example of a dynamic sorption test

**Results and discussion**

The tests were carried out on the powders obtained by grinding samples to 80 μm. In this case, the macroporosity is virtually eliminated and the adsorption takes place essentially in the micropores and mesopores. To study the influence of humidification-drying cycles on the isotherms, we stop the desorption at 10% relative humidity and then proceed the second sorption cycle. The results are presented in Figure 4 for CEM I mortar and in Figure 5 for CEM II mortar. Firstly, we note that the