

# Modelling and Structure/Performance Characterisation of Geopolymer Concrete Containing Encapsulated Phase Change Materials for Thermal Energy Storage in Buildings

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## ABSTRACT

This paper dedicates to investigate the internal microstructure and thermal performance of a thermal energy storage building material, namely geopolymer concrete containing encapsulated phase change materials (GPC-PCMs). X-ray micro-computed tomography (micro-CT) was introduced to characterise the internal microstructure of the proposed concrete material, while the thermal performance of the concrete material was evaluated by a model consisting of micro-CT sample scanning, finite element analysis (FEA) sample modelling and computational fluid dynamics (CFD) thermal simulation. It is found that the PCM encapsulated by dip-coating technique exhibits good quality during concrete mixing and curing. Even PCM distribution and favoured PCM/GPC compactibility were observed in the proposed GPC-PCM sample. In addition, a slightly higher air void content was resulted by the incorporation of PCM. The thermal performance of the suggested concrete material in terms of thermal insulation and thermal energy storage was improved considerably after incorporating the suggested PCM.

**Keywords:** thermal energy storage building material, building operational energy efficiency, geopolymer concrete, phase change materials (PCMs), micro-computed tomography (micro-CT), computational fluid dynamics (CFD) thermal simulation

## 1. INTRODUCTION

Climate change and environmental degradation resulted from energy overconsumption and excessive carbon dioxide (CO<sub>2</sub>) emissions have increasingly aroused concerns in recent years [1]. In the field of civil

engineering, renovation of construction materials plays a vital role in addressing the global threat of climate change and environmental degradation by promoting the concept of sustainable development. Construction and building-related industries are significant contributors to global energy consumption and carbon emissions. In 2017, 36% of global energy consumption was attributed to the building and construction sectors, while energy consumed to maintain the operation of buildings accounted for 30% of the global total [2]. Accordingly, IEA (2018) reports that 11% of the global energy-related CO<sub>2</sub> emissions were released in the heating process of construction material manufacturing (e.g. cement and structural steel production) and construction phase in 2017, and 28% of that was produced through the lifecycle of buildings. Therefore, IEA (2018) describes the buildings and construction sectors as the key actors in the global fight against climate change. Construction material as a crucial participant in the construction industry, improving its sustainability will result in a substantial increase in the overall environmental friendliness and energy effectiveness of the whole project.

The novel construction material investigated in this research is named geopolymer concrete containing encapsulated phase change materials (GPC-PCMs). Geopolymer concrete (GPC), or alkali-activated concrete (ACC), is believed to have a high potential to become the alternative to the conventional concrete that formed by ordinary Portland cement (OPC) [3, 4]. Over the last two decades, researchers in the field of civil engineering materials have been attempting to replace the OPC content in Portland cement concrete (PCC) because its sustainability has been questioned extensively. The manufacture of OPC requires calcination of raw materials

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such as chalk and limestone at a temperature of 1450°C to produce Portland cement clinker [5]. This process is not only energy-intensive but also emit 1.5 billion tons of CO<sub>2</sub> annually recorded in 2014, and the figure was expected to have an increasing rate of 6% in the following years [6]. Compared to PCC, GPC allows a complete replacement of OPC with supplementary cementitious materials (SCMs) in its mixture, in such a way to eliminate the energy consumption and CO<sub>2</sub> emission caused by the heating process in concrete manufacturing.

Besides, the widely used SCMs in GPC, such as silicon fume (SF), fly ash (FA), ground granulated blast-furnace slag (GGBS) and red mud (RM), are by-products of coal, iron and aluminium industries [7, 8]. The utilisation of those industrial by-products not only reduce the negative environmental impacts by diminishing the reliance of the construction industry on OPC. On the other hand, properly sealing those waste materials into constructions can mitigate environmental contamination and free up large areas of land space from storing them [8].

Incorporating phase change materials (PCMs) in concrete is an innovative method to cope with the high operational energy consumption of buildings by taking advantage of PCMs' thermal energy storage property [9]. Latent heat normally refers to the energy required for a substance to change its phase (e.g. solid to liquid). PCMs commonly have a high capacity of latent heat thermal energy storage, which a considerable amount of thermal energy can be stored during the stage of phase change [10]. When the ambient temperature is equal or higher than the melting point of the PCM in the concrete, the chemical bonds of the PCM will break up, and the PCM will transform from solid-state to liquid-state associated with heat absorption from ambience [11]. Correspondingly, a reverse effect will take place after the ambient temperature drops back below the melting point, and a heat release process will be initiated.

In this study, the primary objectives are:

- a. To explore the optimum image reconstruction, refinement, thresholding, segmentation, presentation and exportation methods for the application of micro-CT in microstructure characterisation of GPC-PCM.
- b. To examine the internal microstructures of prepared concrete samples, including the number, size, volume fraction and distribution of air bubbles and PCM pellets, PCM/geopolymer compatibility, as well

as the quality of PCM incorporation through the analysis on micro-CT image data.

- c. To evaluate the thermal energy performance of the proposed concrete sample by determining and comparing the key thermophysical properties of GPC and GPC-PCM samples using CFD thermal simulation.

## 2. MATERIAL AND METHODS

### 2.1 Sample preparation

#### 2.1.1 Materials

The GPC mixture was prepared by mixing low-calcium FA, GGBS and alkaline activator solution (AA) as shown in Fig.1. The FA with the specific gravity of 2.3 g/cm<sup>3</sup> and GGBS with the specific gravity of 2.85 g/cm<sup>3</sup> were purchased from Yuanheng Construction Materials, Henan, China.

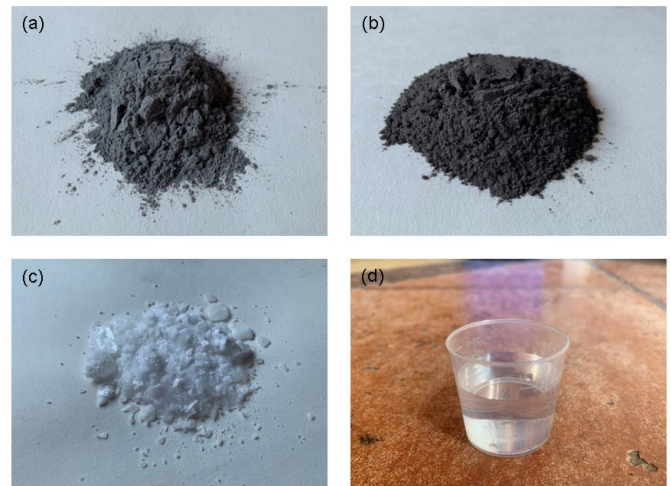


Fig 1 The geopolymer mixing ingredients used in this study, (a) FA, (b) GGBS, (c) solid sodium hydroxide and (d) sodium silicate solution.

AA was prepared by mixing sodium hydroxide (NaOH) solution and sodium silicate (Na<sub>2</sub>SiO<sub>3</sub>) solution with a weight ratio of 2.5 in this study. Sodium hydroxide with the purity of 99% in flake form (Fig 1c) was purchased from Yihua Chemical, Inner Mongolia, China.



Fig 2 Paraffin wax powder used in this study.



Fig 3 Paraffin pellets before coating with geopolymer slurry.

A 12M sodium hydroxide solution was produced by

mixing sodium hydroxide solid with tap water. Sodium silicate solution (Fig 1d) with the silicon dioxide ( $\text{SiO}_2$ ) to sodium monoxide ( $\text{Na}_2\text{O}$ ) mass ratio of 2 ( $\text{SiO}_2 = 29.4\%$ ,  $\text{Na}_2\text{O} = 14.7\%$  and water = 55.9%) was procured from Longgang Chemical, Shandong, China.

Paraffin wax (JouleWax® 28) having the melting point of  $29 \pm 1^\circ\text{C}$ , as shown in Fig 2, was purchased from Joule Wax, Shanghai, China. The physical and thermal properties of the selected paraffin wax were provided by its manufacturer and are presented in Table 1. Obtained paraffin wax powder was melted and reformed into 147 pellets with an average pellet size of 1.5 mm in diameter, as shown in Fig 3. Dip-coating technique was performed by immersing the PCM pellets in geopolymer slurry and leaving them for 6 hours to cure [12]. This process was carried out twice to produce a quality coating (Fig 4).

Table 1 Properties of paraffin wax used in this study.

Appearance	White colour
Form	Dry powder
Density (kg/m <sup>3</sup> )	900
Melting point (°C)	$29 \pm 1$
Thermal conductivity (W/mK)	0.21
Specific heat capacity (J/kg K)	3220
Heat of fusion (J/g)	220
Thermal cycling	Multiple

FA, GGBS and AA were mixed to form the geopolymer paste in this study. The binder material of the mixture was a composite of FA and GGBS with the weight ratio of 7:3 (i.e. FA to binder ratio = 0.7, GGBS to binder ratio = 0.3). AA to binder ratio and water to binder ratio was designed to be 0.35 and 0.14, respectively. There are two methods that commonly used to design the PCM content in the concrete mixing [13]. The first method is the replacement method which is to replace a certain percentage of sand in the concrete mixture with the equal volume of PCMs [13, 14]. The second method is to add PCM into the concrete mixture as an additive directly, and this method is named as the additive method [13, 15]. In this study, the additive method was adopted to design the PCM content. Two  $30 \times 20 \times$

Table 2 Detailed mixing design of samples.

Label	Binder (kg/m <sup>3</sup> )	FA <sup>a</sup> (kg/m <sup>3</sup> )	GGBS <sup>b</sup> (kg/m <sup>3</sup> )	NaOH (kg/m <sup>3</sup> )	Na <sub>2</sub> SiO <sub>3</sub> (kg/m <sup>3</sup> )	AA <sup>c</sup> (kg/m <sup>3</sup> )	Water (kg/m <sup>3</sup> )	PCM <sup>d</sup> (Vol %)
GPC	500	350	150	50	125	175	70	-
GPC-PCM	500	350	150	50	125	175	70	15

<sup>a</sup>Unit weight of fly ash

<sup>b</sup>Unit weight of ground granulated blast-furnace slag

<sup>c</sup>Unit weight of alkaline activator

<sup>d</sup>Volume fracture of phase change material

10 mm samples (Fig 5) were prepared with one plain geopolymer concrete and another one containing 15% of the paraffin wax by volume to form a GPC-PCM. The detailed mixing design of the concrete samples is demonstrated in Table 2.



Fig 4 Paraffin pellets coated with geopolymer slurry.



Fig 5 GPC and GPC-PCM samples at the size of  $30 \times 20 \times 10 \text{ mm}$

## 2.2 Test methods

The explicit descriptions and illustrations of the test procedures for GPC-PCM sample are presented in this section. The test procedures for the GPC sample, including micro-CT data acquisition, image reconstruction, image filtration, image segmentation, geometry exportation, mesh generation and CFD simulation, follows the same workflow as that of the GPC-PCM sample other than the procedures related to the PCM.

### 2.2.1 X-ray micro-computed tomography scanning

The X-ray micro-CT scanning was performed on the two samples by using a Multiscale-Voxel® scanner (Sanying, Tianjin, China) with an accelerating source voltage of 320kV. The volume reconstruction was carried out by using Studio Voxel Recon®. Image filtration was mainly performed in ThermoFisher Avizo®, and the image multi-thresholding and accurate particle separation were conducted based on Top-Hat algorithm and a watershed-based separation algorithm, respectively.

### 2.2.2 Thermal simulation

The thermal simulation was primarily conducted by introducing a model which synthesised by micro-CT sample scanning, FEA sample modelling and CFD thermal



simulation for the thermal performance evaluation. The involved platforms are ThermoFisher Avizo®, Ansys SpaceClaim®, Ansys ICEM®, Ansys Fluent® and Ansys CFD-Post®. A steady-state heat transfer model was set up to evaluate the thermal performance of the proposed concrete sample by determining and comparing its thermophysical properties.

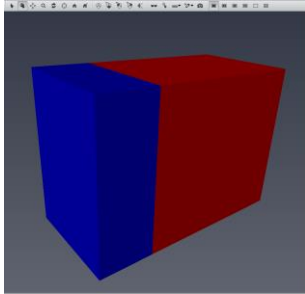


Fig 6 A 40×30×20 mm air domain (red) attached on the bottom of the concrete samples (blue).

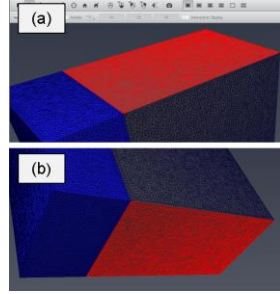


Fig 7 (a) A velocity inlet surface and (b) a pressure outlet surface highlighted in red.

In order to simulate the one-direction steady-state heat transfer condition, a  $40 \times 30 \times 20 \text{ mm}$  air domain was attached to the bottom of the concrete samples by using ThermoFisher Avizo® to create free convection environment, as shown in Fig 6. Then, the boundary conditions were defined as a heat exchange surface (the outer face of the concrete sample), a velocity inlet surface (Fig 7a), a pressure outlet surface (Fig 7b) and seven adiabatic surfaces (the rests).

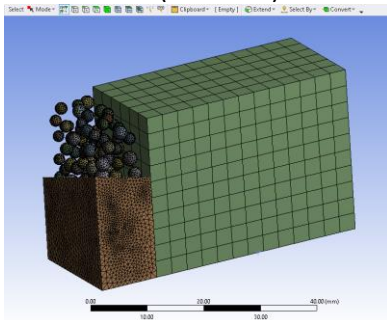


Fig 8 Refined sample mesh by using Ansys ICEM, the upper half of the geopolymer mesh is hidden.

Next, the sample models were then exported to Ansys ICEM® to manually refine the mesh (Fig 8) so that the mesh is in the optimum fashion for CFD simulation. By the completion of the mesh improvement, the models were then ready to be exported to the Ansys Fluent to test their thermophysical properties.

### 3. RESULTS AND DISCUSSION

#### 3.1 Internal Microstructures

Through the analysis of the obtained micro-CT images, an adequate level of evenness can be found in the distribution of the particles inside the concrete sample (Fig 9). Apart from that, as shown in Table 3, the total particle number (i.e. PCM pellets and air bubbles) in the GPC-PCM sample is 282, while the total number of the PCM pellets is 147 which is consistent with the number of the incorporated PCM pellets. The obtained volume fraction using micro-CT scanning is 14.6%, and this percentage is very close to the designed volume fraction (15%). In addition, a low discrepancy between the obtained equivalent spherical diameter (ESD) and designed diameter of PCM pellets is observed. All the findings above indicate that high accuracy can be achieved by using micro-CT scanning combined with the proposed image process methods and the suggested PCM encapsulation technology possesses adequate strength. Moreover, the clear and smooth edges of the PCM pellets (Fig 10) without evident PCM breakage and leakage implicate good compatibility between the incorporated PCM pellets and the geopolymer paste.

Compared to the number of air bubbles between two concrete samples, the number of air bubbles in the plain GPC sample (235) is significantly higher than that in the GPC-PCM sample (135). However, the average particle size of the air bubbles in the GPC-PCM (273.30  $\mu\text{m}$  ESD) is evidently higher than that of the air bubbles in the plain GPC sample (213.41  $\mu\text{m}$  ESD). As a result, the volume fraction of the air bubbles in the GPC-PCM sample (0.11%) is slightly higher than that in the GPC sample (0.09%), despite the less geopolymer paste content in the GPC-PCM sample. That could be a sign of that the incorporation of PCM will most likely induce the higher air void content. A similar result was reported by Pilehvar et al. [16].

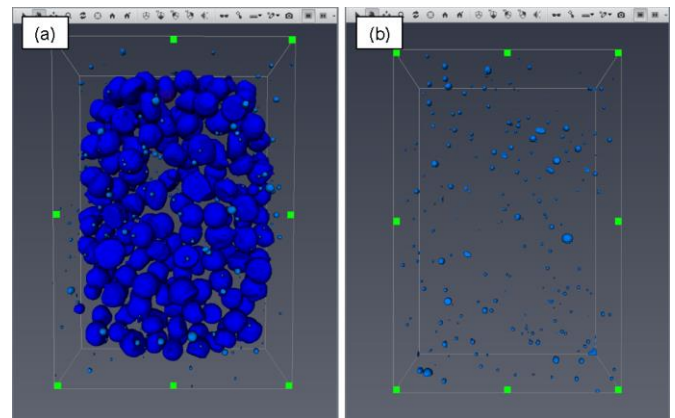


Fig 9 The distribution of the air bubbles (light blue) and the PCM pellets (dark blue) in (a) the GPC-PCM sample and (b) the plain GPC sample.

Table 3 Summarised geometrical information of particles inside the concrete samples.

		GPC-PCM		GPC
		Detected	Incorporated	Detected
Total number of particles		282	-	235
Number of PCM pellets		147	147	
Volume of PCM pellets (um <sup>3</sup> )	Avg	5.84E+09	-	-
	Total	8.76E+11	9.00E+11	-
	Volume fraction	14.6%	15%	-
Surface area of PCM pellets (um <sup>2</sup> )	Avg	1.74E+07	-	-
ESD of PCM pellets (um)	Avg	1,637.04	1,500.00	-
Number of air bubbles		135	-	235
Volume of air bubbles (um <sup>3</sup> )	Avg	4.81E+07	-	2.29E+07
	Total	6.49E+09	-	5.36E+09
	Volume fraction	0.11%	-	0.09%
Surface area of air bubbles (um <sup>2</sup> )	Avg	6.37E+05	-	3.56E+05
ESD of air bubbles (um)	Avg	273.30	-	213.41

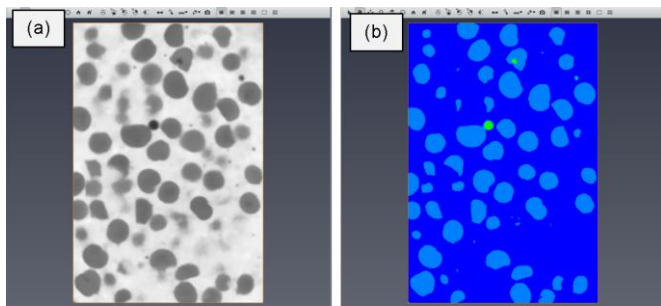


Fig 10 (a) An original ortho slice image, and (b) the image after processing with multi-thresholding to illustrate the PCM pellets in light blue and the air bubbles in bright green.

### 3.2 Thermal performance

The thermophysical properties of the proposed GPC-PCM sample are demonstrated in Table 4. It is found that by incorporating the PCM pellets into the GPC paste, the thermal conductivity of the concrete sample is reduced by 8.51%, whereas the specific heat capacity is increased by 48.70%. The similar trends were presented by Shadnia, Zhang and Li [17] and Cao et al. [18]. Moreover, the most significant change can be observed in material enthalpy, the enthalpy of the concrete sample soar from 9097.49 K/kg to 47086.75 K/kg by incorporating PCM, which reveals a substantial increase of latent heat thermal energy storage capacity of the concrete sample.

Table 4 Obtained thermophysical properties of the concrete samples.

Sample name	Thermal conductivity (W/mK)	Specific heat capacity (J/kg K)	Enthalpy (K/kg)
GPC	0.47	770	9097.49
GPC-PCM	0.43	1144.98	47086.76
Variation rate (%)	-8.51	48.70	418.58

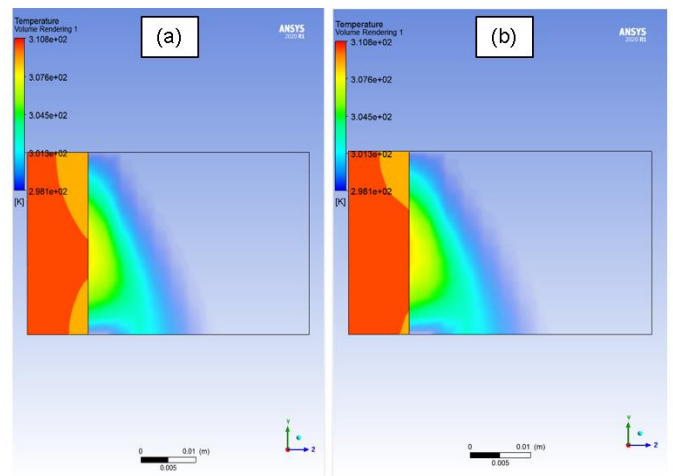


Fig 11 Temperature contours of steady-state heat transfer simulation on the y-plane for (a) the GPC-PCM sample and (b) the plain GPC sample

Furthermore, Fig 11 presents the steady-state heat transfer contour of two concrete samples on the y-plane. It is evident that the inner surface of the GPC-PCM sample shows a relatively lower average temperature than that of the plain GPC sample indicated by the larger orange area on the top-right and bottom-right corners of the GPC-PCM sample. The temperature difference between the inner surface of GPC sample and GPC-PCM

Table 5 Average temperature on the inner surfaces of the concrete samples.

Sample name	Average temperature on concrete inner surface (°C)
GPC	37.15
GPC-PCM	34.24
Difference	2.91
Variation rate (%)	-0.08

sample is 2.91 °C, as shown in Table 5. The value changes of the all three thermophysical properties and the inner surface temperatures between two samples provide the convincing evidence that the thermal insulation and thermal energy storage properties of the GPC sample were improved considerably by integrating the proposed PCM. A comprehensive comparison and analysis of the influence of incorporating PCM to the indoor air temperature fluctuation will be carried out using the transient-state heat transfer simulation model in the following research.

#### 4. CONCLUSION

This study mainly concerns the enhancement of the operational energy efficiency in building sectors by developing an thermal energy storage building material named GPC-PCM. In order to cope with the agglomeration issue of microencapsulated PCM, selected PCM was incorporated into GPC by dip-coating method on the mesoscale. A novel examination method by using X-ray micro-CT scanning was introduced to characterise the internal microstructures of the prepared samples without any destruction done to the samples in advance. In addition, the thermal energy performance of the proposed GPC-PCM was evaluated through a model synthesised by micro-CT sample scanning, FEA sample modelling and CFD thermal simulation.

The key findings of this study are summarised as follows:

- a. Examining the internal microstructures of GPC-PCM based on the obtained micro-CT images and the proposed image processing techniques demonstrates high-level accuracy.
- b. Encapsulating the selected PCM by dip-coating technique shows adequate quality indicated by no significant breakage and leakage after the concrete curing process.
- c. Even PCM distribution and favoured PCM/GPC compactibility were observed in the prepared concrete sample.
- d. Incorporating PCM into GPC could lead to a slightly higher air void content taking into consideration of the less geopolymer paste content in the GPC-PCM sample. That might contribute to the strength reduction of the GPC-PCM compared to the plain GPC.
- e. The thermal energy performance of GPC elements in terms of thermal insulation and thermal energy storage can be evidently enhanced by incorporating suggested PCM according to the results achieved in the steady-state heat transfer simulation.

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