Numerical simulation of the effects of a Phase Change Material (PCM) on solidification path of gravity sand cast Al-Cu alloy

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Solidification structure has a significant effect on mechanical and physical properties of metallic materials and its control is a main direction in the research for the improvement of materials performance. Various methods, such as control of cooling rate, inoculation, imposing vibration and pressure, are traditionally used to control the solidification structure during casting and solidification processes. In this paper, the preliminary results of a new method for controlling the solidification structure during casting using Phase Change Materials (PCMs) are presented. The evolution of the solidification structure of a directionally chilled Al-Cu alloy poured in a silica sand mould with and without the use of pure zinc as a PCM was examined using experimental and simulation methods. It was shown that the PCM temperature could reach about 510 °C during the solidification of the aluminium alloy, therefore, absorbing its melting latent heat from the solidifying aluminium alloy melt which affects its local solidification cooling rate. Therefore, the solidification structure of the sample cast in the PCM fitted mould differed from that of the sample without PCM. While macrostructures of both samples showed the transition from columnar to equiaxed grains, the columnar zone in the PCM sample was larger than in the sample without PCM. In other words, columnar to equiaxed transition (CET) for the sample without PCM occurred sooner than that for the sample with PCM. In addition, the average size of the equiaxed grains at the Chill sample is smaller than the PCM sample.

KEYWORDS: MACROSTRUCTURE CONTROL, GRAVITY SAND CASTING, PHASE CHANGE MATERIALS (PCMS), COLUMNAR TO EQUIAXED TRANSITION (CET)

INTRODUCTION

Aluminium casting alloys have huge applications in automotive, sport, and aerospace industries because of such special properties as excellent thermal and electrical conductivity, appropriate castability, reasonable weldability, lightweight and good corrosion resistance [1, 2]. It has been established that different processing parameters including cooling rate [3], application of electric and magnetic fields [4] and directional solidification [5] can affect the casting macro and microstructure as well as the solidification path. Using metal or graphite chillers is another way to control the final casting structure as well as to produce castings with minimum shrinkage defects. Different types of chiller materials such as copper, iron, or aluminium based alloys as well as graphite can be used according to their heat capacities and diffusivities. It is obvious that each of these materials can absorb and transfer a specific amount of heat before saturation by heat. Therefore, both type and dimen-

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sions of chillers have an important role on heat transfer, cooling rate, and solidification microstructure of the castings [6]. Obviously, larger chillers are required for higher heat absorption, and the areas closer to the chill experience higher cooling rates resulting in the formation of fine columnar microstructures [7].

In this paper, a new way to control the solidification macrostructure of metallic alloys by using Phase Change Materials (PCMs) is proposed. PCMs are materials that can absorb or release their latent heat at a relatively constant temperature (their melting temperature) during the solid-liquid transition [8]. PCMs are mainly used in such applications as buildings [9] and solar systems [10] to save heating energy. In this study, a PCM has been incorporated into a metal chiller and its effect on the cooling and solidification macrostructure of a directionally solidified Al-Cu alloy is investigated using experimental and simulation methods.

EXPERIMENTAL PROCEDURE
ALLOY AND CASTING METHOD

Al-4.5wt.%Cu-0.2wt.%Fe alloy, low carbon steel and commercially pure zinc were considered as the poured metal, chiller and PCM, respectively. Schematics of the casting moulds are illustrated in Fig. 1. The moulds were made of sodium silicate bonded silica sand. The casting dimensions were $30 \times 30 \times 70$ mm^3. In order to provide enough time for

melting of the PCM (pure Zn) during solidification of the Al-Cu alloy and to further encourage directional solidification of the castings, alumina insulation (not shown in the figure) was used around the casting cavity.

The Al-Cu alloy was melted and superheated to 750 °C in a graphite crucible using a resistance furnace and cast in two moulds fitted either with a chill (Chill sample) or with PCM (PCM sample), as shown in Fig. 1. In the Chill sample, a solid chiller with $30 \times 30 \times 13$ mm^3 dimensions was placed at the end of the casting. In the PCM sample, a steel container with $30 \times 30 \times 25$ mm^3 dimensions and wall thickness of 2 mm filled with pure zinc was used. In order to evaluate the effects of the latent heat absorption of the PCM on the cooling rate and solidification structure of the Al-Cu alloy, dimensions of the PCM and the encasing box were selected in a way that they had the same cooling power as that of the solid chiller up until the melting of the PCM.

For recording the temperature during the pouring and solidification of the alloy, three K-type thermocouples were located in the castings at 10, 35 and 60 mm from the chill surface. One thermocouple in the chiller (in the Chill sample) and two thermocouples in the PCM (in the PCM sample) were also employed (Fig. 2). The temperature data was collected using a data acquisition system with a sampling rate of 1 s^{-1}, analog-to-digital converter accuracy of 0.1°C, which was linked to a personal computer.
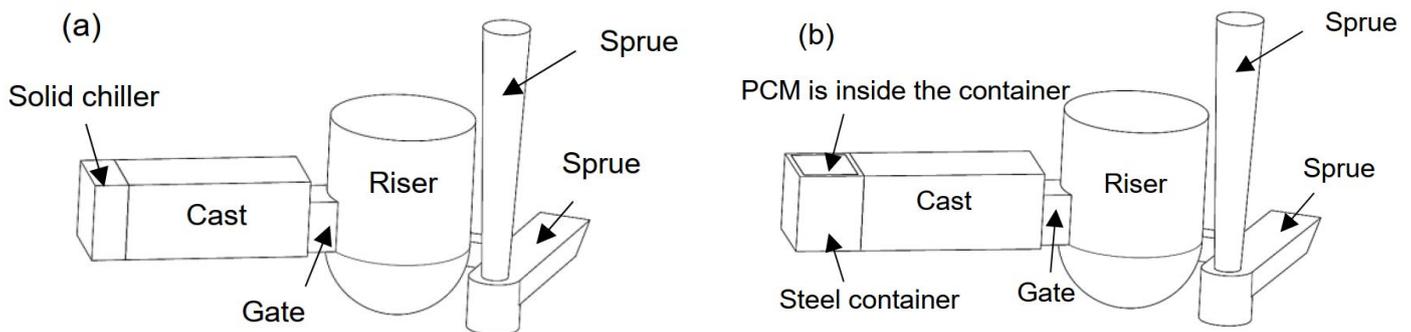
Fig.1 - Schematics of the casting moulds: (a) Chill sample and (b) PCM sample.

MACROSTRUCTURE INVESTIGATION

In order to study the macrostructure of the castings, longitudinal sections of the cast samples were ground by silicon carbide (SiC) papers to 600 grit and etched with Keller etchant (1.5 ml HCl, 2.5 ml HNO$_3$, 1 ml HF and 95 ml distilled water).

CASTING SIMULATION

Before casting, the optimum mould designs were obtained based on numerical simulation with ProCast 2018 software. Tetrahedral mesh number was chosen 209517 for the casting, 17078 for the chiller, 43510 for the steel container, 71214 for the PCM, 124499 for the runner system, 285639 for

the insulator and 431920 for the mould. The heat transfer coefficients were selected according to Tab. 1. The mass flow was selected at 200 g/s.

Tab.1 - Heat transfer coefficients (HTC) between different interfaces of the moulds.

	Cast-Chill	Cast-Insulator	Cast&Runner-Mould	PCM-Chill	Insulator-Mould	Chill-Mould
Chill sample	4500-5500	200	900	---	50	600
PCM sample	8000-10000	200	1000	9000-15000	50	800-1000

RESULTS AND DISCUSSION
EXPERIMENTAL RESULTS

Fig. 2 demonstrates the collected experimental temperature-time (T-t) curves of both Chill and PCM samples at different positions. According to Fig. 2, for the Chill sample, all the thermocouples in the casting rapidly reached 750 °C and then were cooled gradually. The chiller temperature also reached 600 °C. On the other hand, for the PCM sample, the temperature reaches about 600 °C at 10 and 35 mm from the chill surface before dropping down suddenly and rising again to 600 °C in less than 100 s. Then they continue a gradual cooling process. At 60 mm from the chill surface, the temperature reaches 750 °C, then cools down to about 650 °C where it remains almost constant for about 150 s and then starts to decrease. The differences among the curves at the early stages of the casting are thought to be related to the turbulence of the melt during metal pouring when the molten metal may touch the thermocouples temporarily. Furthermore, the T-t curves of two positions inside the PCM

is shown in Fig. 2. It shows that the PCM temperature at position Zn1 reaches the melting point of the pure zinc, i.e. 419.5 °C, after 11 s and finally reaches about 510 °C after 40 s. The PCM temperature at position Zn2 reaches its melting point after 30 s and finally increases to about 500 °C after 120 s. The latent heat absorption effect of the PCM is evident in the curve corresponding to Zn2. According to Fig. 2, at the early stages, the PCM sample has cooled faster than the Chill sample because of the effect of PCM melting.

The thermophysical properties of zinc are different from steel. The specific heat coefficient of pure zinc, at both solid and liquid phases, is less and its heat conductivity is more than steel [11, 12]. Therefore, the heat transfer in the PCM sample would be more than that in the Chill sample, resulting in a faster temperature drop in the PCM sample. Moreover, when the pure zinc starts to melt at the early stages, it absorbs its latent heat from the Al alloy. This extra heat absorption is believed to affect the cooling rate and, consequently, the macrostructure of the aluminium alloy casting.

(a)

(b)
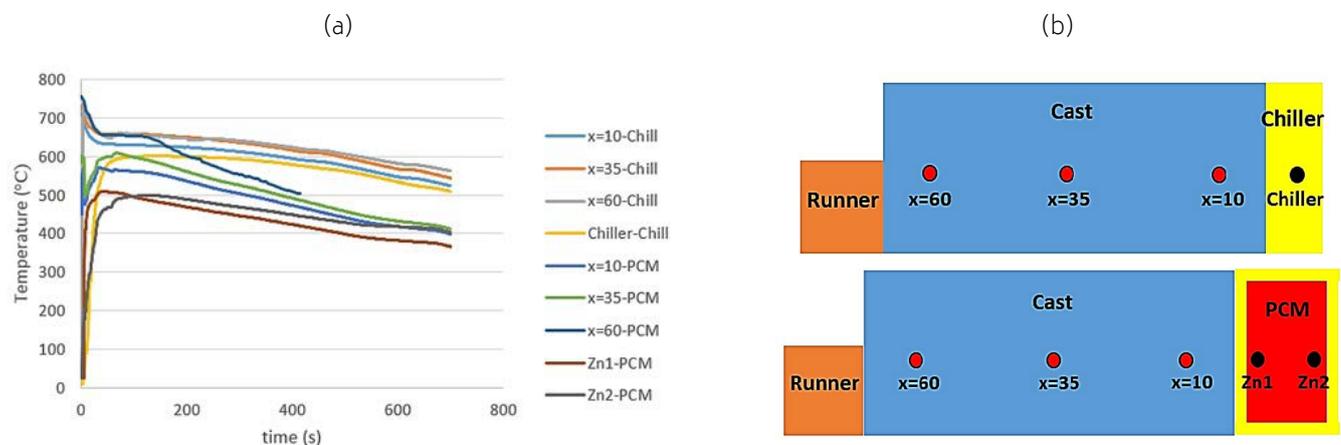
Fig.2 - (a) Experimental T-t curves for both PCM and Chill samples and (b) Location of three thermocouples at 10, 35, and 60 mm from the chiller surface in both PCM and Chill samples, one thermocouple in the chiller (Chill sample) and two thermocouples, i.e. Zn1 and Zn2, in the PCM (PCM sample).

Fig. 3 illustrates the macrostructures of both samples. Each macrostructure consists of a columnar structure grown on the chill surface followed by an equiaxed grain structure towards the ingate of the casting. A clear CET (Columnar-Equiaxed Transition) is observed in both castings. Length of columnar regions, measured using ImageJ analysis software, is equal to about 38 and 41 mm for Chill and PCM samples, respectively.

According to Fig. 3(a), a distinct difference between the two macrostructures is that solidification in the chill sample appears to has started from the lower corner of the steel chill and the columnar grains have grown towards the upper surface of the Chill sample. On the other hand, all the columnar grains grew uniformly perpendicular to the chill surface in the PCM sample with a direction opposite to that of the heat transfer. The difference is believed to be related to the air gap between the PCM and the steel container. In the Chill sample, when the molten metal first touches the lower part of the solid steel chiller during pouring, an intense heat transfer sets in, resulting in rapid nucleation and growth of grains from the contact area. The total chilling capacity of the solid chiller is concentrated on this small contact area. Due to the large volume of the chiller, it is not easily saturated by the transferred heat. As a result, the grains grow in the opposite direction to the heat transfer. Therefore, these localized nucleation and heat transfer phenomena at the lowest corner of the chiller have determined the grain orientation of this sample.

In the PCM sample, however, the PCM is encapsulated in a 2 mm thick steel container. When the molten metal comes in contact with the steel chiller, the PCM cannot effectively participate in the heat transfer at the beginning due to the presence of an air gap between the PCM (pure Zn) and the steel chiller. Therefore, the steel container wall heats up quickly avoiding a localized heat transfer from the first contact points.

The air gap is practically removed when the encapsulated PCM melts. Melting of the PCM, on the one hand, increases the heat transfer between the casting and the chiller/PCM assembly and, on the other hand, absorbs its latent heat from the casting. As a result, the cooling rate of the PCM sample increases and its solidification time decreases resulting in a larger columnar zone compared to those of the Chill sample, as shown in Fig. 4. The average size of the equiaxed grains was calculated by the lognormal distribution method [13]. According to related equations, the average grain sizes are 1.8 ± 1.3 mm and 2.2 ± 1.8mm for the Chill and PCM samples, respectively.

Previous researches have shown that by determining the thermal gradient (G) at the solid-liquid interface and the solid-liquid interface velocity (R), it is possible to predict the CET formation [14-16]. It has been shown that CET will occur when the G/R ratio decreases and reaches below a critical value. Upon decreasing the thermal gradient in front of the solid-liquid interface, the constitutional undercooling in front of the solidification front increases and equiaxed grains can grow in an unconstrained manner [15]. In this work, the measured amount of G/R (according to the simulated T-t curves) at the time of CET formation was about 14.9 and 0.05 °C·s/cm^2 for the Chill and the PCM samples, respectively. Higher G/R value in the Chill sample means that CET took place at a higher thermal gradient and/or smaller solidification growth. In other words, the formation of CET at the Chill sample is easier than that in the PCM sample. Therefore, in the Chill sample, the equiaxed zone has occurred at a closer distance to the chiller surface, and as a result, has a finer macrostructure.

(a)

(b)
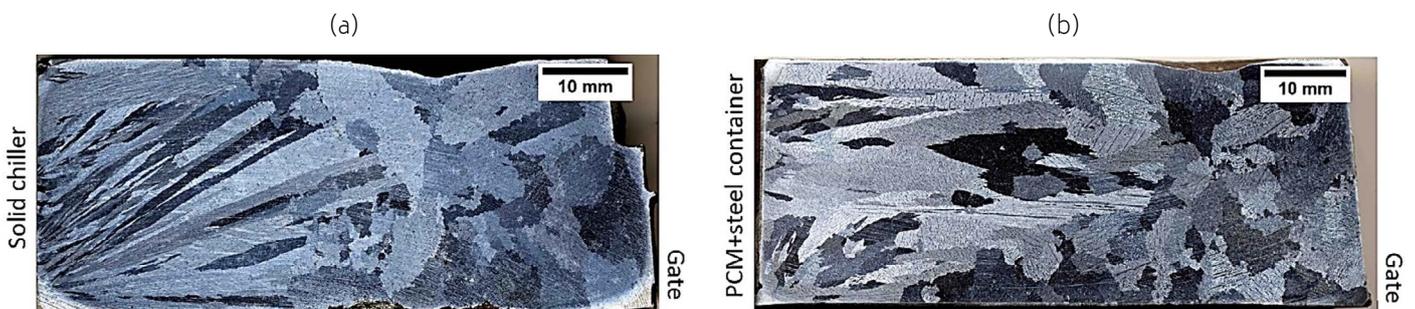
Fig.3 - Macrostructure of (a) Chill and (b) PCM samples.

SIMULATION RESULTS

Figs. 4(a) and 4(b) show the experimental and simulation T-t diagrams of the Chill and PCM samples, respectively. As it is observed, there is a good agreement between the simulation and the experimental data. The cooling rate near the liquidus temperature was measured at different points according to the simulation diagrams in the temperature range of 644-634 °C. The cooling rate at the chiller/casting interface (x=0 mm) for both samples is about 28.6 °C/s suggesting how the dimensions of the chiller and PCM were correctly designed, i.e. they provide a similar chilling effect at the beginning.

At a distance of 10 mm from the chiller, the cooling rate at the mushy zone near the solidus temperature is about 4.6 and 7.7 °C/s for the Chill and the PCM specimens, respectively. At greater distances (x=35 and x=60 mm), the cooling rates in the PCM sample are even larger than those in the Chill sample. These differences are thought to be due to the presence of the PCM (pure zinc), i.e. because of different physical properties in comparison to solid steel chiller and its melting at the early stages of casting solidification. As a result, the chilling powers in both samples were similar before melting the PCM, but the cooling rate and solidification conditions changed after melting the PCM.
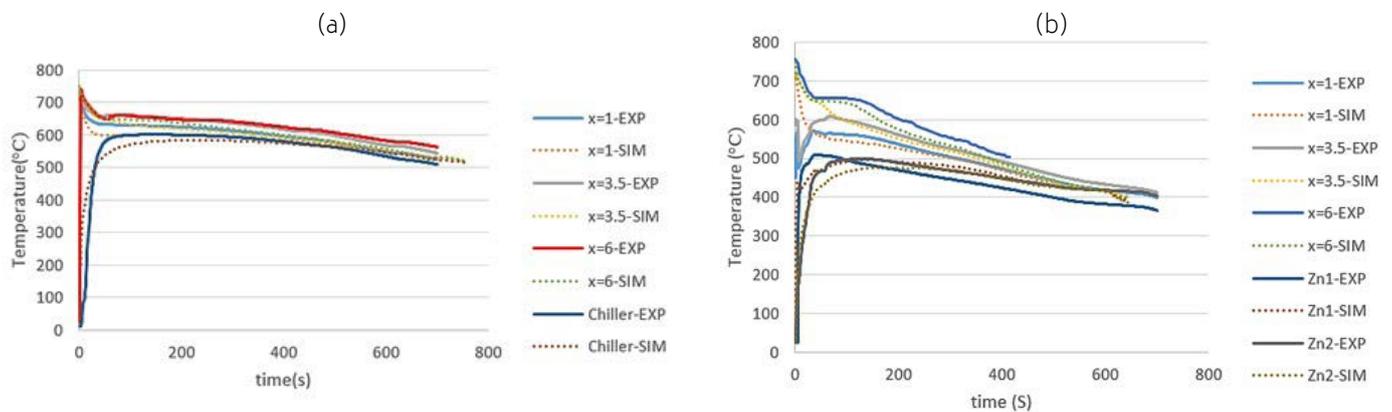
Fig.4 - Experimental and numerical cooling curves for (a) Chill and (b) PCM samples.

CONCLUSION

In this paper, a novel method to control the solidification macrostructure of an Al-Cu alloy using Phase Change Materials (PCMs) was studied using experimental and simulation approaches. The results showed that the incorporation of a zinc PCM into a metal chiller affected the cooling and solidification conditions of a directionally solidified Al-Cu alloy. Columnar to Equiaxed Transition (CET) was observed in both samples. However, it occurred later for the sample fitted with the zinc PCM. The effects are believed to be due to absorption of the latent heat of melting of the PCM during the early stages of solidification of the casting as well as the different thermophysical properties of the PCM and chill materials. Based on the results, the proposed method can be used as an innovative cooling system to control the solidification macrostructure of the castings.

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