

NUMERICAL INVESTIGATION OF SOLIDIFICATION BEHAVIOR OF AL-4.5CU ALLOY USING A ZN–GRAPHITE FOAM COMPOSITE PCM CHILLER

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<https://doi.org/10.37904/metal.2026.5265>

Abstract

A composite chiller consisting of graphite foam infiltrated with pure zinc as a phase change material (PCM) and enclosed within a steel container was used to enhance heat transfer and accelerate the solidification of an Al-4.5 wt% Cu alloy. Cooling performance was evaluated using numerical simulation based on temperature-time diagrams, along with calculations of thermal gradient (G) and growth rate of the solidification front (R). The results were validated through comparison with available experimental data related to pure zinc as PCM and to conventional steel chillers. The results indicate that the porous foam structure increased the effective surface area and reduced the volume-to-surface ratio, enabling earlier melting of zinc and improving its heat absorption from the molten alloy. The Zn–graphite foam composite enhanced heat extraction during the early stages of solidification, reducing the solidification time compared to the other types of chillers. This promoted an ideal temperature distribution within the completely filled mould cavity, making the subsequent cooling path favourable to feeding. Higher thermal gradients were observed near the composite chiller. In all configurations, G/R decreased from the chiller toward the runner, indicating the potential for a columnar-to-equiaxed transition (CET); however, this reduction was more abrupt in the composite case, suggesting shorter columnar growth and accelerated CET. Consequently, a more equiaxed microstructure with reduced shrinkage defects is expected. Despite using less zinc, the high thermal conductivity of the graphite foam compensated for this reduction, demonstrating the superior efficiency of the Zn–graphite foam composite chiller.

Keywords: Phase Change Material, Composite chiller, Thermal gradient, Cooling rate, Controlled solidified structure

1. INTRODUCTION

Aluminium alloys are extensively used in various applications such as in the aerospace and automotive industries, due to their high ductility, excellent formability, corrosion resistance, and good electrical and thermal conductivity [1]. Numerous methods have been proposed to control the solidified structure and, consequently, the final properties of these alloys. These methods include grain refinement [2], semi-solid casting [3], cooling rates control [4], and directional solidification [5].

Directional solidification is particularly effective for producing single crystals as well as polycrystalline structures with reduced shrinkage defects, especially in regions close to the chiller. It is important to note that different types of chillers are employed in foundries, including external or internal chillers [6], as well as chillers used in continuous casting processes [7].

Recently, a new generation of chillers using a phase change materials (PCMs) has been introduced to influence the macro- and microstructure of aluminium alloys [8]. In this approach, a PCM is a material with a constant melting temperature that melts during the solidification of the cast alloy, absorbing latent heat from the metal [9]. This enables greater heat absorption at a nearly constant temperature, thereby enhancing the cooling capacity of the chiller. It has been observed that this type of chiller reduces the solidification time and

minimizes casting defects, such as microporosity, compared to conventional chillers. In addition, it can accelerate the columnar-to-equiaxed transition (CET) [8].

Graphite chillers have attracted significant attention due to their high thermal conductivity and are widely recognized as effective cooling materials in foundry applications. In the present study, to further enhance the heat absorption capacity of the chiller, a composite structure consisting of graphite foam infiltrated with pure zinc, acting as a phase change material (PCM), was developed. For comparison, a chiller of identical dimensions made of pure graphite was also considered. Both configurations represent novel approaches and were initially investigated through numerical simulations. The results were subsequently compared with previously reported experimental and numerical data to evaluate their accuracy and performance.

2. MATERIALS AND METHOD

In this study, an Al–4.5 wt% Cu alloy containing 0.35 wt% Fe as an impurity was cast using silica sand moulds. A composite chiller, consisting of a porous graphite material infiltrated with pure zinc as a PCM, was placed inside a steel container with 2 mm thickness. For comparison, a pure graphite chiller was also employed. **Figure 1** illustrates the 3D geometry of the components within the sand mould, along with the shapes and dimensions of the different chillers.

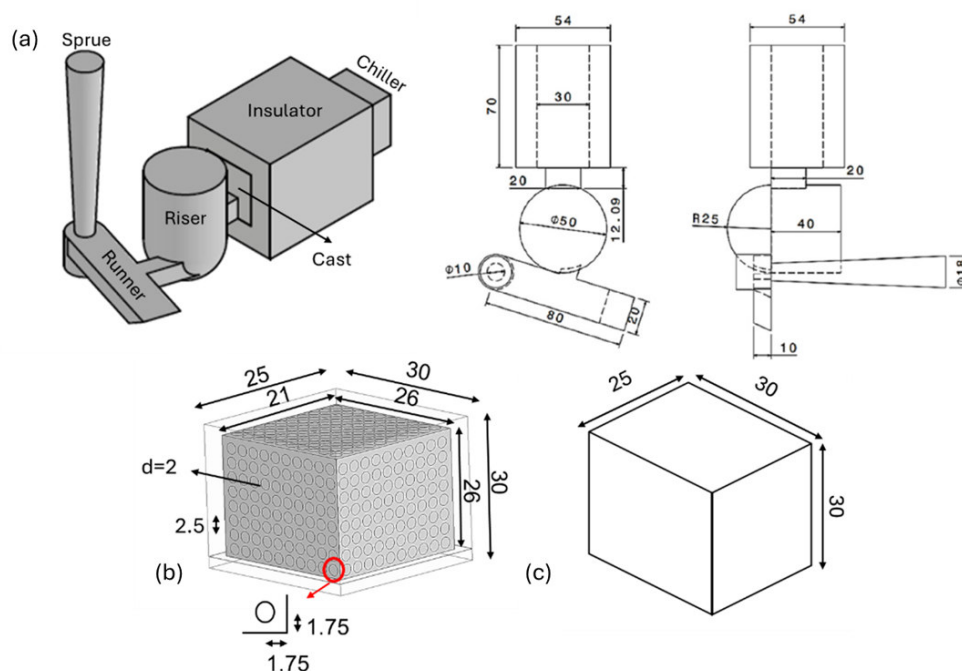


Figure 1 Schematic illustration and dimensions of (a) 3D geometry of mould parts, (b) Zn-graphite foam composite chiller inside of steel container with 2 mm thickness and (c) graphite chiller.

This study focuses exclusively on numerical simulations. The results were validated against experimental and numerical data from a previous work [8], conducted using similar processing conditions. The commercial software ProCast[®] (2021 version) was used to investigate the cooling performance of the proposed chillers.

The thermophysical properties, including melting temperature, thermal conductivity, specific heat capacity, density and thermal diffusivity, for sand mould, insulator, alloy and chillers were sourced from the software database. For the graphite used in the chillers, the thermal conductivity, specific heat capacity and density were set to 174.5 W·m⁻¹·K⁻¹, 670 J·kg⁻¹·K⁻¹ and 1,890 kg·m⁻³, respectively [10].

Mesh sensitivity analyses were preliminary carried out, and the optimum tetrahedral meshes for newly introduced materials were determined as follows: 3,042,845 cells for pure zinc, 1,383,134 cells for graphite foam, and 112,112 cells for cubic graphite. The heat transfer coefficients (HTCs) at the interfaces of foam-PCM, foam-container, graphite-mould, and graphite-alloy were set to 7,000-9,000, 8,000, 100, and 8,000-10,000 W·m⁻²·K⁻¹, respectively. The mesh for the remaining parts and the HTCs between other interfaces were defined according to ref. [8]. It should be noted that perfect thermal contact between the foam and the PCM was assumed, with full interfacial contact considered throughout the composite domain. The pouring temperature and the melt inlet flow rate were set to 750 °C and 200 g·s⁻¹, accordingly. Furthermore, the Cellular Automaton–Finite Element (CAFE) module of numerical simulation software was used to predict the macrostructure, grain size, and columnar zone length of the castings. Subsequently, the equiaxed grain size, and the columnar zone length obtained from the CAFE model were compared with the experimental data obtained by using an optical microscope equipped with Leica application suit (LAS) image analyser.

The simulation results were utilized to determine the thermal gradient (G) and the growth rate (R) of the solidification front. These evaluations were conducted along the central longitudinal axis of the casting. Temperature-time ($T-t$) profiles were recorded at uniform 1 mm intervals, extending from the chiller surface to the gating system, resulting in 71 measurement points for each sample. Average G and R values were calculated at 10 mm increments using these data. For each selected position, the precise moment the temperature reached the liquidus temperature of the Al–4.5 wt.% Cu alloy was first identified. At this specific time, the temperatures of the subsequent nine nodes (spanning a 10 mm distance) were extracted. From these values, temperature–distance ($T-x$) curves were constructed, and the thermal gradient (G) ahead of the solidification front was determined from the slope of these curves. The growth rate (R) at each position was then calculated by:

$$R = \frac{10}{\Delta t} \quad (1)$$

where Δt represents the time interval between the moments when the first and the last nodes within each 10 mm segment reached the liquidus temperature.

3. RESULTS AND DISCUSSION

3.1 Thermal and solidification simulations

Figure 2 illustrates the $T-t$ curves of both castings at various positions. **Table 1** presents the thermal gradient (G) and the solidification velocity of the solid/liquid interface (R) across different regions of the castings. The casting with the composite chiller exhibited a steeper slope than the casting with graphite chiller. As shown in **Figure 2a**, the pure zinc within the graphite melted at approximately 420 °C, and its temperature increased to about 500 °C after nearly 200 s. In contrast, the temperature of the cubic graphite reached around 600 °C within 50 s (**Figure 2b**). Consequently, the graphite chiller became thermally saturated more rapidly, after which its temperature decreased concurrently with the cooling of the alloy. According to **Table 1**, the cooling rate ($G \times R$) of the casting with the composite chiller in regions near the chiller was higher than that of the casting with graphite chiller. Due to the significantly increased surface-to-volume ratio of the graphite foam, a higher initial cooling rate was achieved. The extracted heat was distributed throughout the foam structure, leading to an increase in the zinc temperature. However, the presence of an air gap between the zinc and the foam slightly reduced the heat transfer efficiency, resulting in a localized decrease in the cooling rate in the 10–20 mm region. Once zinc melting began, latent heat absorption enhanced the heat extraction capacity of the composite chiller, leading to an increase cooling rate and a more pronounced influence on the solidification behaviour of the cast alloy. In contrast, the graphite chiller, despite its high thermal conductivity, rapidly

reached thermal saturation due to its limited heat storage capacity. Consequently, its ability to extract heat diminished quickly, leading to lower sustained cooling efficiency compared to the composite system.

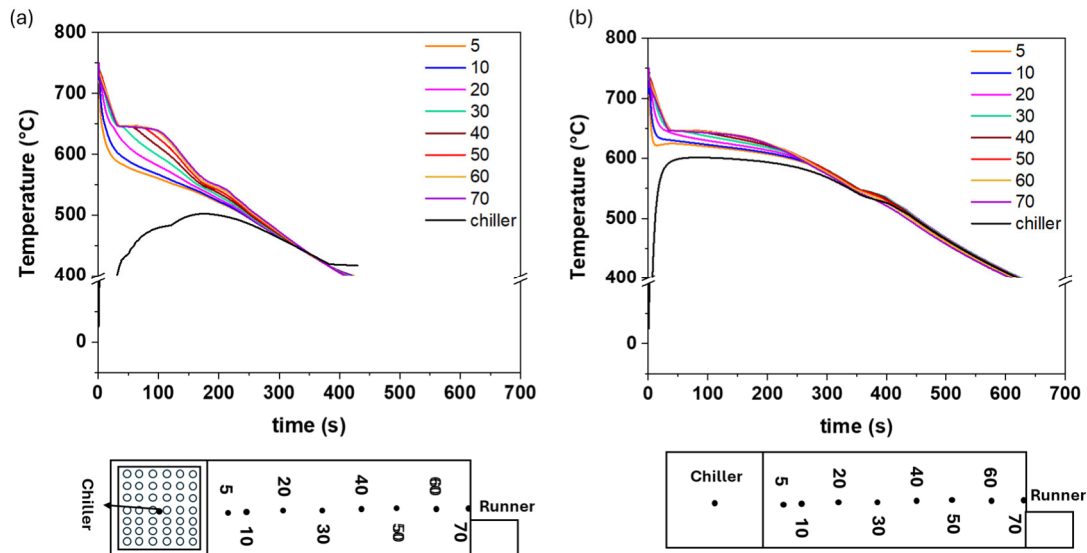


Figure 2 T-t curves at various positions along the central cross-section of castings obtained using (a) composite and (b) graphite chillers.

The solidification times were 236 s and 416 s for the castings obtained using the composite and graphite chillers, respectively. As a result, the composite chiller demonstrated superior cooling performance compared to the graphite one. Accordingly, it is anticipated that the casting produced using the composite chiller will exhibit significantly lower microshrinkage porosity compared to the casting obtained with the graphite one.

Table 1 Solidification parameters for both castings obtained using composite and graphite chillers.

X (mm)	G (°C·mm ⁻¹)		R (mm·s ⁻¹)		G/R (°C·s·mm ⁻²)		G×R (°C·s ⁻¹)	
	Composite	Graphite	Composite	Graphite	Composite	Graphite	Composite	Graphite
0 - 10	8.67	8.58	1.06	0.98	8.15	8.75	9.23	8.41
10 - 20	2.97	3.29	0.81	0.82	3.65	4.01	2.41	2.69
20 - 30	1.18	0.68	0.94	0.68	1.25	1	1.11	0.47
30 - 40	0.04	0.02	2.38	0.58	0.02	0.03	0.11	0.01
40 - 50	0.0002	0.001	10	0.57	0.00002	0.001	0.002	0.0003
50 - 60	-0.003	-0.001	10	2.04	-0.0003	-0.0003	-0.03	-0.001
60 - 70	-0.26	-0.25	1.60	0.33	-0.17	-0.76	-0.42	-0.08

These results were compared with previously reported experimental and simulation data for castings produced using a conventional steel chiller and a new generation chiller consisting of pure zinc as a PCM inside the steel container with 2 mm thickness (**Figure 3**). As it is observed in **Figure 3a**, the T-t curve of the casting obtained using the graphite chiller lied above all other samples, followed by the casting produced by conventional steel and PCM chiller at a distance of 10 mm from the chiller inside the casting, while the casting with composite chiller exhibited the lowest curve. The T-t curves at the 60 mm position (**Figure 3b**) showed that nearly all castings started to solidify at similar temperature; however, the casting with the composite chiller reached to the solidus temperature sooner than the others. As shown in **Figure 3c**, the maximum temperature of a conventional steel chiller was approximately 550 °C, while the temperature of pure zinc used as a PCM

reached about 500 °C after melting. The T–t curves of the casting with composite and pure zinc chillers were in close agreement at all positions up to the temperature range between the solidus and liquidus temperatures. Beyond this range, the slope curve of the casting with composite chiller became significantly steeper than that of the casting with the pure zinc as a chiller. Despite the lower amount of zinc in the composite chiller (approximately 11,007 mm³ compared to 14,196 mm³ in the PCM sample), the incorporation of graphite foam with high thermophysical properties effectively compensated for this reduction. As a result, the melting of zinc occurred more rapidly, leading to a more pronounced effect on the solidification time and microstructure, leading to a shorter solidification time compared to the other samples and a more pronounced influence on the final microstructure of the casting.

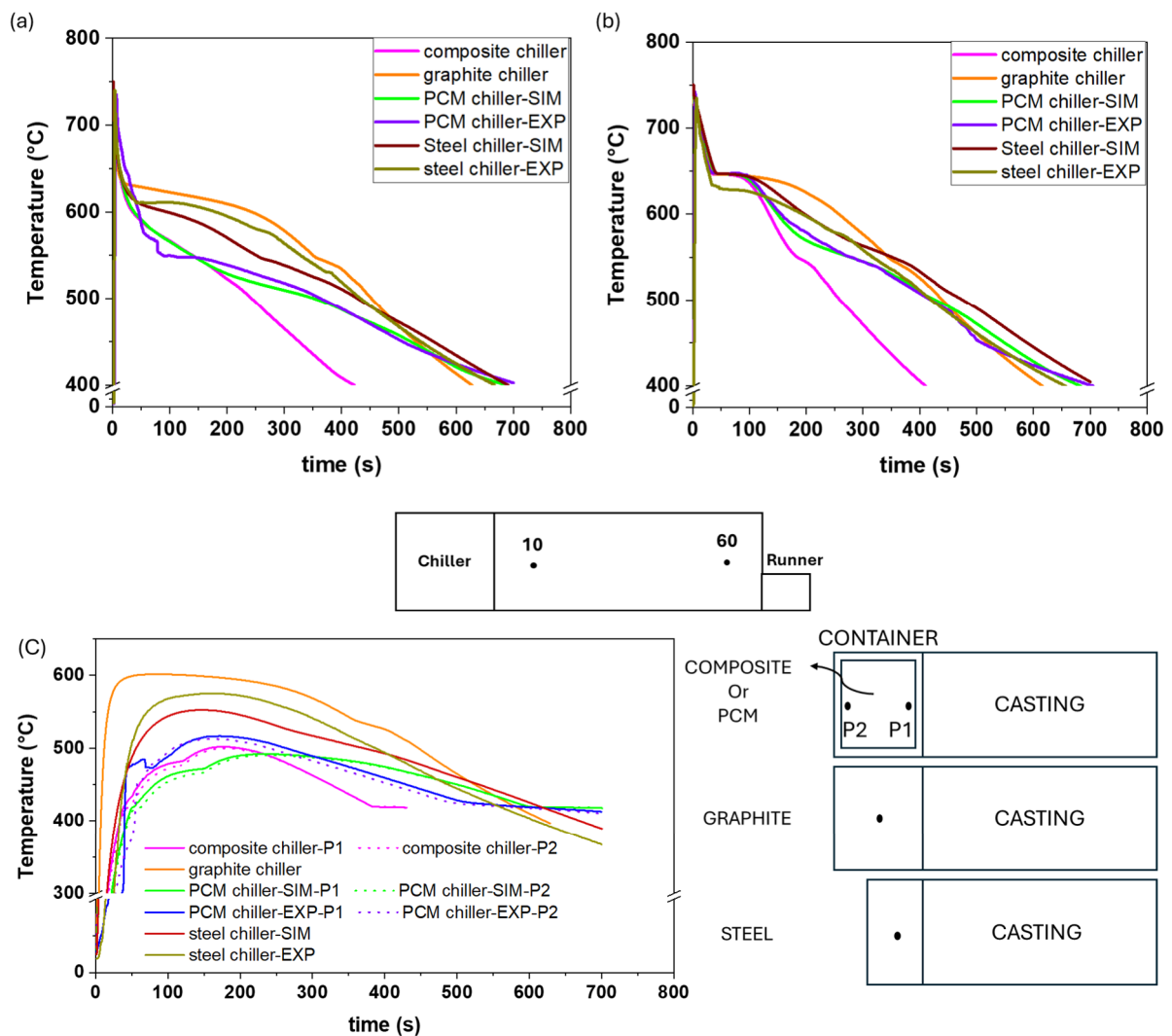


Figure 3 T–t cooling curves for castings produced using various chiller types, recorded at distances of (a) 10 mm and (b) 60 mm from the chiller interface; (c) T–t profiles within the chillers at the designated positions.

3.2 Columnar-to-equiaxed transition

According to **Table 1**, the thermal gradient (G) in the casting produced with the composite chiller was generally higher than in the one obtained using the graphite chiller, except in the 10–20 mm region. In this zone, both the thermal gradient (G) and cooling rate ($G \times R$) of the former were slightly lower than those of the latter, indicating a consistent trend. In directional solidification, due to the high heat transfer near the chiller, columnar grains typically grow opposite to the direction of heat flow. However, the formation of equiaxed grains is

generally preferred, as it leads to improved isotropy of mechanical properties. Hunt [11] proposed an important criterion for predicting the occurrence of the columnar-to-equiaxed transition (CET) based on the G/R ratio evaluated in different regions of the sample. A decrease in the G/R value from regions close to the chiller toward those farther away promotes the formation of equiaxed grains. The G/R values for both castings decreased from the chiller toward the runner as shown in **Table 1**.

Figure 4 shows the CAFE simulation results for both castings. The results indicated that the columnar zone length in the castings produced using composite and graphite chillers was approximately 18.1 mm and 17.8 mm, respectively. The equiaxed grain size, calculated using the LAS image analyser, was 2.3 ± 0.8 mm and 2.5 ± 0.8 mm for the castings obtained with composite and graphite chillers, respectively. Despite the marginal difference, the consistently shorter solidification time suggested that the composite chiller limits solute segregation during solidification of the casting. This results in a more homogeneous chemical composition and a lower incidence of microshrinkage defects in the final component. On the other side, the CET in the casting produced with PCM and steel chillers occurred at distances of approximately 35 and 48 mm from the chiller, respectively [8]. This indicates that the graphite chiller was more effective than the conventional steel one, as the CET occurs earlier and the solidification time was reduced. Even though the CET in the casting produced with the graphite chiller occurred earlier than in the casting with PCM, the overall soundness of the casting must also be considered. Despite the delayed CET, the shorter solidification time induced using the PCM chiller may lead to reduced casting defects. In contrast, the composite chiller demonstrated superior performance; it is expected that a greater amount of finer equiaxed grains is formed, along with improved casting soundness. Overall, the composite chiller exhibited the higher effectiveness among all investigated chilling systems.

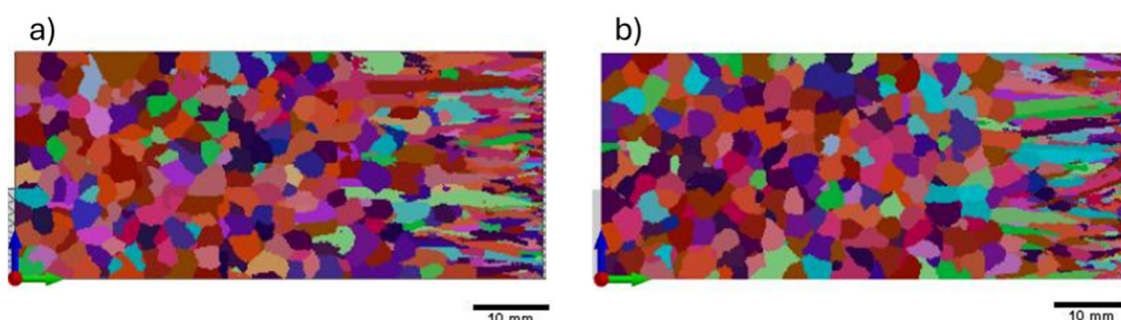


Figure 4 Simulated macrostructure obtained using the CAFE model of castings produced with (a) composite and (b) graphite chillers.

4. CONCLUSION

The conclusions of this study can be summarized as follows:

- The composite chiller exhibits superior cooling performance compared to graphite, pure zinc as a PCM in the container, and conventional steel chillers.
- The combination of graphite foam and latent heat absorption of zinc enhances the overall heat extraction capacity.
- The columnar-to-equiaxed transition (CET) occurs earlier in both casting with composite and graphite chillers, leading to a shorter columnar zone in comparison to the castings produced using PCM and conventional steel chiller.
- Reduced solidification time in the casting with composite chiller can limit the solute segregation and decrease microshrinkage defects.
- The composite chiller improves both the thermal conditions and the microstructural quality of the casting.

ACKNOWLEDGEMENTS

This work was developed with the financial support of the Strategic Department Investment (SID2024) within the Project “Innovative PCM-based chillers to tailor the solidification structure of recycled light alloys”.

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