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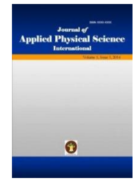

MICRO-MACRO MODELLING OF SOLIDIFICATION WITH EXPERIMENTAL VALIDATION IN SELECTED EUTECTIC BINARY ALUMINIUM ALLOYS

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AUTHORS' CONTRIBUTIONS

This work was carried out in collaboration among all authors. Author HEM designed the study, performed the statistical analysis and wrote the first draft of the manuscript. Author CPE formulated the boundary conditions, wrote the MATLAB codes and performed the computer simulation. Author GMS conducted the experiments for the various mould and made the temperature measurements. Author GIL supervised the research and managed the literature review. All authors read and approved the final manuscript.

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ABSTRACT

Experimental and numerical studies of solidification phenomena have continued to complement each other in the quest for advanced knowledge during component manufacture. The dynamics of engineering designs coupled with the desire for lightweight and improved materials have sustained the progress achieved in recent decades on the modelling of casting systems. The current study presents the simulation of solidification conditions for different aluminium-based eutectic binary alloys and validation with an experimental investigation. The effect of mould material was analysed for the solidification of Al-4.5% Cu using metallic, sand, quartz and Plaster of Paris (POP) moulds respectively. Simulation of the eutectic alloys was carried out using micro-macro model previously developed by the current authors. The effect of mould size and transient evolution of structure during solidification in static casting process were successfully simulated. The results of the experimental investigation showed that although the cooling curves for the different mould materials are qualitatively similar, they respond differently to the presence of the liquid metal leading to significantly different rates of latent heat evolution. The simulated cooling curves for the four eutectic alloys solidified inside sand mould showed that Al-4.5% Cu and Al-3.0% Si have the fastest transformations while Al-6.0% Mg and Al-3.0% Zn have the slowest rate of cooling. Mould size has significant influence on thermal distribution during solidification as temperature tends to reach steady-state and homogenize faster in smaller moulds than bigger ones. For all the alloys compared, nucleation period is very small relative to the total solidification time. The results showed that transient evolution of volumetric grain density and grain radius varied significantly.

Keywords: Simulation; micro-macro modelling; solidification; eutectic binary alloys; experimental validation.

1. INTRODUCTION

Solidification is a key phenomenon of engineering importance because majority of the processes involved in the manufacturing of components (especially metal alloys) undergo solidification at one point or the other. The formation of the solidification microstructure of alloys depends on the specific

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casting technique which directly influences their mechanical and physical properties. Experimental investigations into in-situ structural evolution during solidification of metal alloys have proved to be difficult, time consuming and expensive. Complementing experiments with numerical modelling and simulation has lessened the burden imposed by these disadvantages mentioned above. Modelling and simulation have also deepened the knowledge of heat transfer, fluid flow and structure formation during casting. Additionally, more complicated geometries that were hitherto difficult for experimental studies have been successfully studied with numerical methods. The mechanical properties of cast alloys generally depend on the physical metallurgy of the solidification microstructures such as grain size, morphology, distribution and the presence of insoluble eutectics. These factors can be manipulated by considering appropriate solidification conditions or modification of the solidifying interface morphology.

Several experimental studies involving special casting techniques and electromagnetic effect of solidifying aluminium alloys [1-6] have been reported. Kanaujiya and Taiwari [1] conducted experimental investigation on solidification rate and grain size for centrifugal casting. They deployed magneto-hydrodynamics (MHD) and electromagnetic stirring to study the casting velocity and its effect on macro-segregation. Fan and Liu [2] studied the solidification behaviour of AZ91D alloy under intensive forced convection in the rheo-diecasting (RDC) process. They used this casting process which is relatively new semisolid approach for the production of near net shape component to study the solidification behaviour of AZ91D alloy. This is to understand the effects of forced convection, shearing time and shearing temperature on the nucleation and growth behaviour. They reported that under intensive forced convection, heterogeneous nucleation occurred continuously throughout the entire volume of the solidifying melt. It was also found that due to uniform temperature and composition field created by the forced convection, most of the nuclei could survive the solid-liquid interface disturbance such as thermal fluctuations. The nuclei were observed to grow spherically with greatly fast growth rate. In another study [3], grain refinement effect of pulsed magnetic field on solidified microstructure of superalloy IN718 was presented. They showed grain refinement effect under pulsed magnetic field (PMF). Nowak et al. [7] studied grain refinement effect of Nb-B inoculant on the Al-Si alloys through the analysis of binary Al-xSi alloys. The evaluation of the microstructure and the thermal behaviour of the binary Al-xSi alloys showed that the Nb-B inoculation is highly suitable for Al-Si alloys with Si content greater than 6wt%. As a result, both the α-grains and the eutectic phase are significantly refined. Kaygisiz and Marash [8] presented the effect of growth rates on microhardness, electrical properties and microstructure for directionally solidified Al-13wt% Mg_2Si pseudoeutectic alloy at a constant temperature gradient. Bridgman type of directional solidification furnace was used in the directional solidification process comparing five growth rates at a constant temperature gradient. The microstructure of the alloy was observed to be Mg_2Si coral-like structural phase dispersed into the primary α-Al phase matrix. The dependency of the microhardness and electrical resistivity on growth rates were quantified.

Hajkowski and Ignaszak [9] combined both experiment and computer simulation to evaluate the impact of casting conditions on the microstructure and mechanical properties of AlSi9Cu3. The correlation between the parameters of structure and mechanical properties were established. In order to observe microscopic details of structure evolution during casting processes, solidification phenomena are studied at different length scales. Hamilton et al. [10] coupled macroscopic and microscopic levels of modelling to simulate the casting process over a wide range of spatial and temporal scales. This yielded multiscale model where micromodels for dendrite arm spacing and microporosity were incorporated into a macromodel of heat transfer. Their model was applied to investment casting of aluminium alloys. Micro-macro modelling of solidification behaviour of metals and alloys has been developed as a second generation of computer simulation to predict the actual development of microstructure during the production of components. Some of these models [11-14] assume eutectic solidification and that thermal undercooling play dominant role in the evolution of structure during the eutectic transformation. They used specific nucleation and growth laws to track solid fraction as solidification progresses. Experimental results and published data are the most accurate data used to validate the results predicted from modelling and simulation exercise. Such direct comparisons of experimental and numerical results have been presented by many studies [15-17]. Majority of the most technologically important eutectic alloys consist of two phases [18]. Solidification phenomena and microstructure evolution of several eutectic alloy systems have continued to attract more research and industrial interests. This is because eutectic alloys exhibit good properties and performance under service conditions [19]. The aim of the current study is to validate the previously presented micro-macro model [14] and to use the model to analyse transient evolution of microstructure during solidification of different aluminium-based eutectic binary alloys.

2. MATERIALS AND METHODS

2.1 Casting of the Samples

The materials used for patternmaking, mould-making and the preparation of the alloy include: quartz mould, sand mould, POP mould, mild steel plate for the metallic mould, gmelina wood, binders (water and clay), parting line powder, mould boxes, hand blower, spade, trowel, riddles, rammers, vent wire, head-pan, digital weighing balance, Aluminium (99.3% purity) sourced from First Aluminium (Nig.) Plc Port-Harcourt, Nigeria copper (99.5% purity) sourced from Cutis Cables Plc, Nnewi, Nigeria, thermocouple (Centre 309 datalogger), computer.

The casting setup used to produce the metal alloys is shown in Fig. 1. Different castings were produced using rectangular moulds made of quartz, sand, POP and metal (mild steel). The size of each of the casting is 200 mm x 100 mm x 50 mm. The total charge for each was 3,300 kg of Al-4.5% Cu alloy. Graphite crucible was used to melt the alloy while charcoal provided the melting heat. The system was superheated to 720^{o}C to ensure good casting fluidity. The temperature measurements were taken using center309 datalogger digital thermometer whose model is TP-K01 bead probe. It is a four channel digital thermometer that is instrumented with K-type thermocouples as temperature sensors. It has internal memory that can keep up to 16,000 records per channel and uses RS232 interface to perform bi-directional communication with the computer. The numerical display screen uses four digital liquid crystal display (LCD) per channel while its operating range of temperature is between -200°C and 1370°C. The actual measurement was made by probing the thermocouples into the solidifying melt and interfacing same to a computer. The reference position for all the casting was the centre of the ingot. The instrument takes temperature reading at every two seconds. At the end of each casting, the cooling curve data were exported from the datalogger and were converted to excel file and later exported to *MATLAB* where the cooling curves were plotted for different mould materials. Casting experiments were conducted to study the effect of mould materials on the solidification of Al-4.5%Cu eutectic binary alloy. Metallic, silica sand, quartz sand and POP moulds were used for the experiments. To ensure the same melt-thermal conditions within the mould cavities, no mould was preheated and pouring was done at 720^{o}C for each casting.

Fig. 1. Experimental casting setup for the production of the alloys

2.2 Numerical Modelling

The cavity of the casting domain being modelled is a rectangular geometry (200 mm x 100 mm x 50 mm) as shown in Fig. 1. The detailed problem formulation for the domain consisting of model assumptions, boundary conditions and heat transfer regimes within the solidification system has been presented in a previous article by the authors [14-15]. The micro-macro model was built based on continuous nucleation model and is applied in the current work to study transient evolution of microstructures in Al-4.5 wt.% Cu, Al-6.0wt.% Mg, Al-3.0 wt. % Si and Al-3.0wt.%Zn eutectic binary alloys. The effect of mould size on the solidification of these alloys is also modelled and the results are presented in the subsequent sections. Heat transfer in this work is dominated by conduction and hence the advection term in the transport equation is ignored. The energy equation as presented by [14 & 15] is given as

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right) + \dot{Q} \quad (1)$$

Where T is the temperature, t is time, k is the thermal conductivity, ρ is the density, c_p is the specific heat at constant pressure, $\dot{Q}$ is the volumetric source term associated with the phase change and it determines the rate of latent heat evolution during liquid-solid transformation attributed to solidification in the absence of convection. The finite volume method of Patankar [20] was used to discretise Eq. 1. The volumetric source term which is the last term on the right hand side of Eq. 1 was treated using solidification kinetics. The details of the mathematical modelling, thermo-physical properties data, solidification kinetics constants and implementation of the solution technique are explicitly presented in [14].

3. RESULTS AND DISCUSSION

3.1 Experimental Result Analyses

Fig. 2 shows the cooling curve plots for various castings obtained with different mould materials. The cooling curves of Al binary alloys with different mould materials are qualitatively similar. However, the observed quantitative variations in the cooling curves are due to the differences in the thermo-physical properties of the mould materials. These materials respond differently to the presence of the liquid metal and therefore rate of evolution of the latent heat varied significantly. A close observation shows that the metallic mould had the fastest cooling rate when compared to other moulds. With the same time of casting, the cooling in metallic mould reached almost 500 K. A value that is far lower than those obtained from other moulds. It can also be seen that the metallic mould has the shortest isothermal phase transformation range. It can further be observed that the isothermal period for the metallic mould is more of a straight line. These differences are attributed to the superior thermal properties of the metallic mould in comparison with the other mould materials. The cooling curves produced by sand and quartz mould materials are both qualitatively and quantitatively similar. This is primarily due to the closeness of their thermal behaviours as the latent heat content of the melt evolved at similar rate for the two materials. They have the same isothermal phase change period. At the same total time of solidification, their temperature is similar at 650 K which is far higher than the value obtained from metallic mould. The POP mould has the poorest heat extraction rate and has the longest isothermal solidification period, even though the isotherm is not straight. This shows that the POP mould can hold latent heat for a longer time compared to other mould materials.

Due to the availability of the thermo-physical property data for the sand mould, the experimental validation of the numerical model will be done for the cooling curve from sand mould. The details for the experimental and numerical validations are presented in the next section.

3.2 Model Validation

It is usually a common practice to validate the results from numerical models with experimentally determined data. This is done to boost the trust and confidence reposed on the results predicted from such models. The micro-macro models are not usually validated against analytical solutions because experimental and numerical data remain the most credible alternatives to validate these models. The results from the current study are validated by comparing the predicted cooling curve with experimental results. The cooling curve from the experiment was used to validate the micro-macro model in Fig. 3. It can be seen from the comparison that the results from both experiment and numerical model are qualitatively similar. The observed quantitative discrepancies especially toward the end of cooling solidification could be as result of discretisation error in the numerical modelling or error from experimental measurement. For instance, the temperature sensors that were used to acquire the experimental cooling curves measure temperature at every 2 seconds while the time step for the micro-macro model was 0.1 seconds. The time step in the model must be small in order to accurately capture microscopic information such as nucleation rate, grain size and volumetric grain density. The sensitivities of the thermocouples in the experimental setup and those in the numerical time stepping may be responsible to the slight discrepancy observed in Fig. 3. However, the observed variation from both methods can be tolerated.

3.3 Numerical Model and Transient Microscopic Evolution

Grid convergence studies were undertaken to ensure that the solutions of the numerical model are independent of the grid size. The details of such grid independence studies as suggested by Celik et al. [21] have been previously presented by the current authors in another report [15].

Fig. 4 shows the results of the grid convergence studies for the four eutectic alloys considered in the current study. It can be seen from Fig. 4a and 4c that the solutions for Al-Cu and Al-Si are more sensitive to grid sizes than those of Al-Mg and Al-Zn as observed in Fig. 4b and 4d respectively. However, these variations from grid sizes can be adjudged to be negligible and therefore the solution is generally said to be independent of grid size. In order to reduce computational time while maintaining good accuracy, the grid size of 4,900 nodes were used in subsequent simulations.

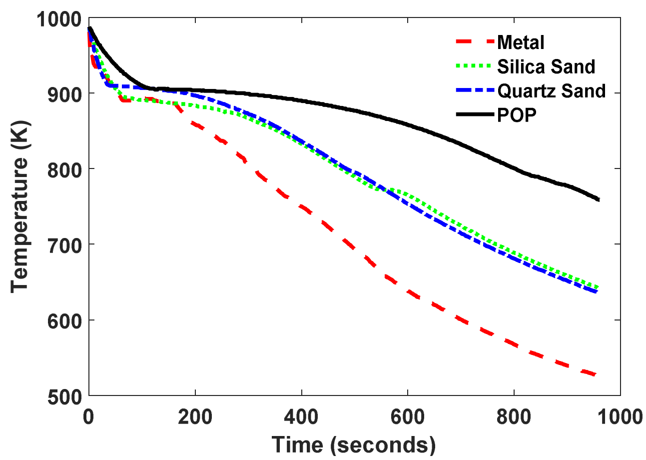

Fig. 2. Experimental cooling curves obtained from different mould materials during solidification

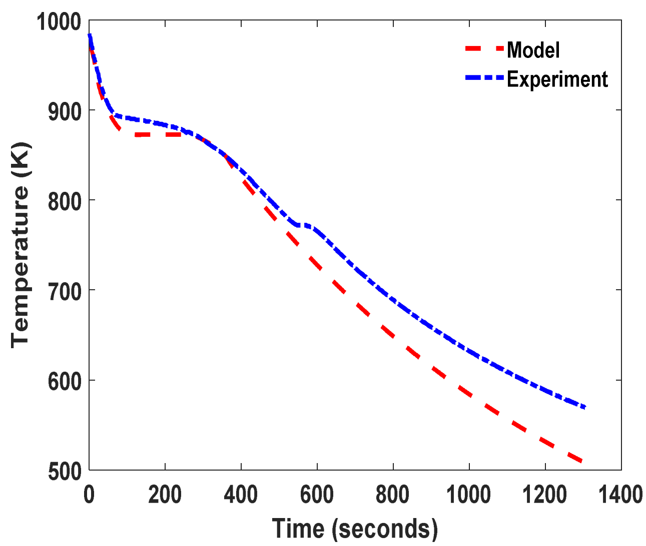

Fig. 3. Cooling curve validation for the micro-macro model using the experimental result

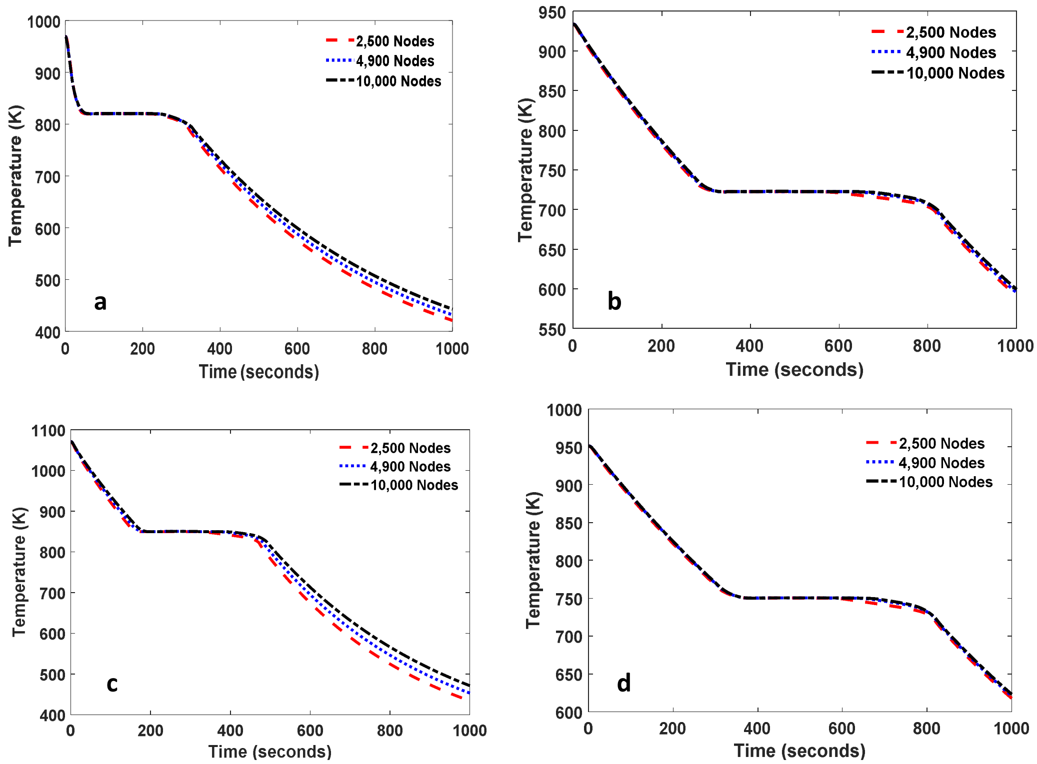

Fig. 4. Grid independence studies for (a) Al-Cu (b) Al-Mg (c) AL-Si (d) Al-Zn alloys

Fig. 5 shows the cooling curves obtained from the four aluminium-based eutectic binary alloys. A close observation of the four cooling curves in Fig. 5 shows that the curves have the same pattern and therefore are qualitatively similar. It can also be seen that the four curves are not entirely the same in terms of cooling rate and length of the isothermal phase transformation period.

Since the simulation conditions are the same for all the alloys considered, these observed quantitative variations in their cooling curves as seen in Fig. 5 can be attributed to the thermo-physical properties of the individual alloys. Al-Cu and Al-Si have the fastest transformations while Al-Mg and Al-Zn have the slowest rate of cooling. It is also seen that the isotherms for the four alloys are similar in their pattern, however, the isothermal length of Al-Mg and Al-Zn are longer than those of Al-Cu and Al-Si as observed in Fig. 5. The cooling curves obtained in Fig. 5 are similar to those reported by previous researchers [11-13].

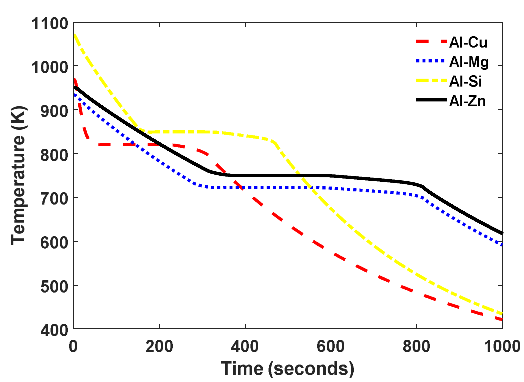

Fig. 5. Predicted cooling curves from the various eutectic aluminium alloys

Fig. 6 shows the effect of mould size on the solidification of different eutectic alloys after 1000 seconds. It shows temperature distribution along the middle horizontal direction within the mould cavity. It can be seen from Fig. 6 that mould size has significant influence on thermal distribution during solidification of eutectic alloys in static casting process. It shows that temperature tends to reach steady-state and homogenize faster in smaller moulds than bigger ones. It can be seen from Fig. 6 that the effect of mould size is not entirely the same for the four eutectic alloys considered. This differential is attributed to the properties of the individual alloys.

Fig. 7 shows the contour of solid fraction for the various alloys after 500 seconds. It describes the solidification front for the various eutectic alloys. The sharp yellow region represents the solidified region while the deep blue area represents the liquid zone. Between the fully solid and liquid regions, there are two other regions called slurry and mushy zones. The light blue and dark yellow layers represent the slurry and mushy regions respectively. Due to the superior thermal properties of the Al-Cu system, more regions have solidified compared to other systems. As a result, the slurry and mushy zone layers of the Al-Cu alloy are larger than those of the counterpart alloys as observed in Fig. 7.

The nucleation rates for the alloys are compared in Fig. 8. It shows that for all the alloys compared, nucleation period is very small relative to the total solidification time. This supports the assumption of instantaneous nucleation models [11-13]. However, it can be seen from Fig. 8 that nucleation started at different times for the various eutectic alloys. It can also be observed that the higher the thermal conductivity of the alloy, the narrower is the nucleation period.

Figs. 9 and 10 show the transient evolution of solid fraction against grain size and the combined volumetric grain density and grain size respectively for all the eutectic alloys. Time evolution for the

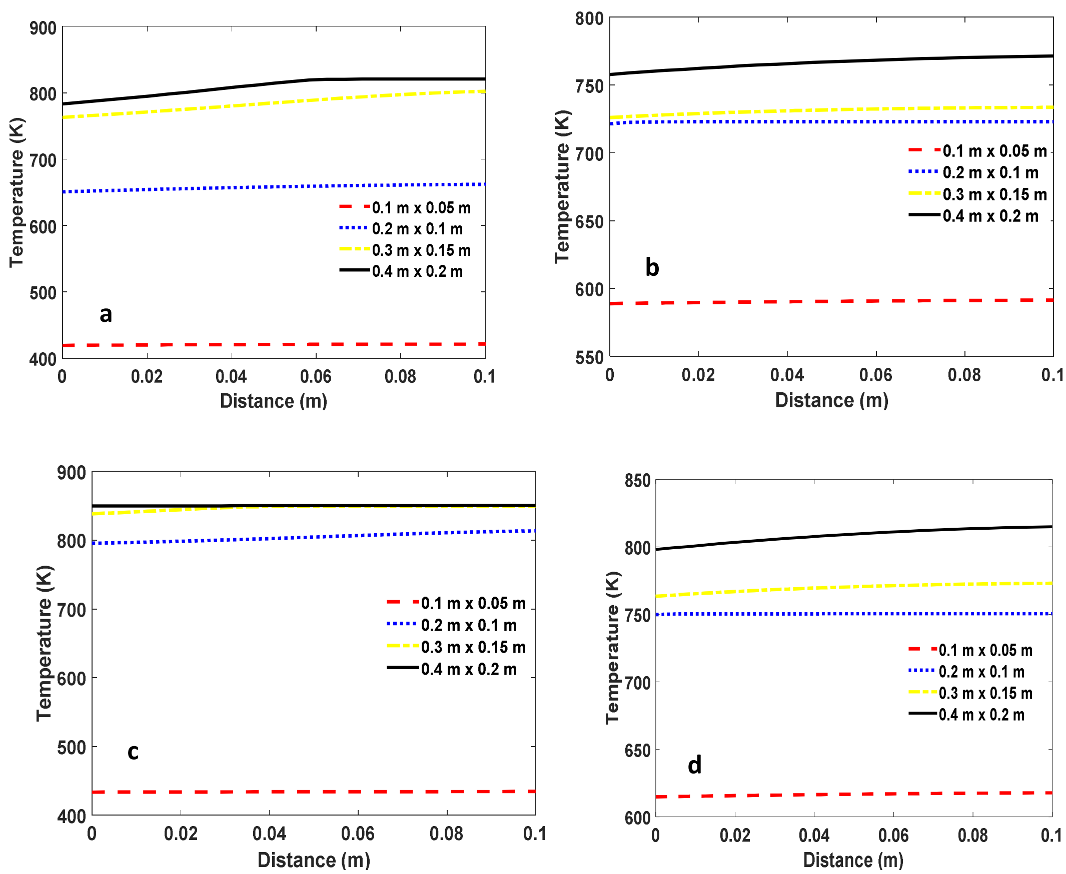

Fig. 6. Effect of mould size on solidification for (a) Al-Cu (b) Al-Mg (c) Al-Si (d) Al-Zn

microstructures shown in Figs. 9 and 10 varied for the different eutectic alloy systems. Fig. 9a-c show transient evolution of grain size as a function of solid fraction for Al-Cu system from 100 sec to 300 sec. At 100 sec, grain size increases with increasing solid fraction as shown in Fig. 9a. At 260 sec, grain size has reached maximum value and grain coherency will occur at this point. The remaining liquid within the interdendritic and inter-eutectic regions will solidify by coarsening while the grain radius remains constant. Fig. 9c shows constant grain radius on further solidification to 300 seconds. Similar transient evolution of volumetric grain density and grain radius are shown in Fig. 10a-c. It took longer times for other systems to reach grain coherency and maximum volumetric grain density as shown in Figs. 9 and 10. Al-Si system was simulated between 300 and 400 seconds. At 300 seconds, grain density and grain size are still increasing as seen in Figs. 9g and 10g respectively. At 360 seconds, these values have reached maximum values as observed in Figs. 9h and 10h. On further solidification, both grain size and volumetric grain density remain constant as shown in Figs. 9i and 10i. Time evolution of microstructure for Al-Mg and Al-Zn are similar and are shown in Figs. 9d-9f, 9j-9l, 10d-10f and 10j-10l. The observed differences in their periods to reach grain coherency and maximum volumetric grain density are also attributed to the significant difference in the thermo-physical properties of the alloys.

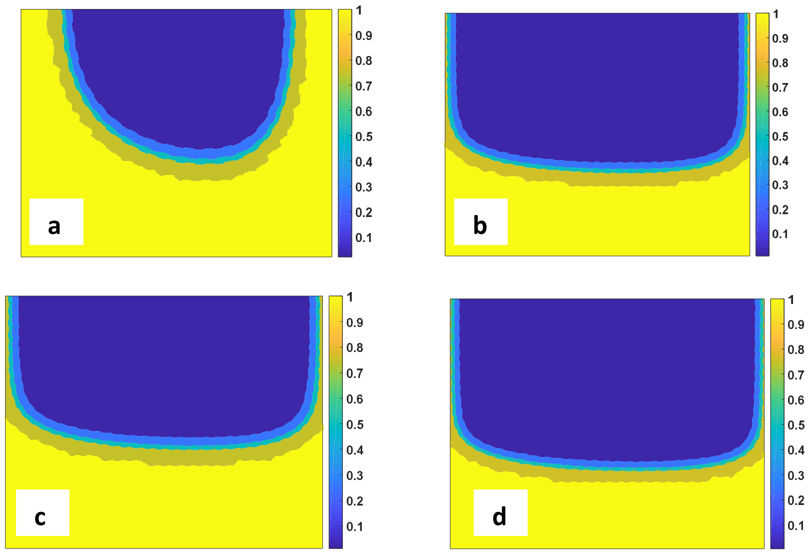

Fig. 7. Contour of solid fraction at 500 seconds for (a) Al-Cu (b) Al-Mg (c) Al-Si (d) Al-Zn

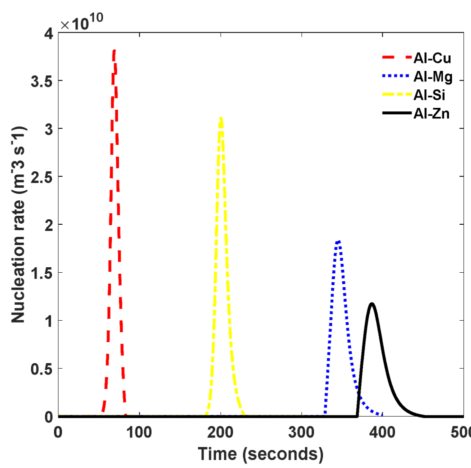

Fig. 8. Rate of nucleation for Al-Cu, Al-Mg, Al-Si, and Al-Zn eutectic alloys

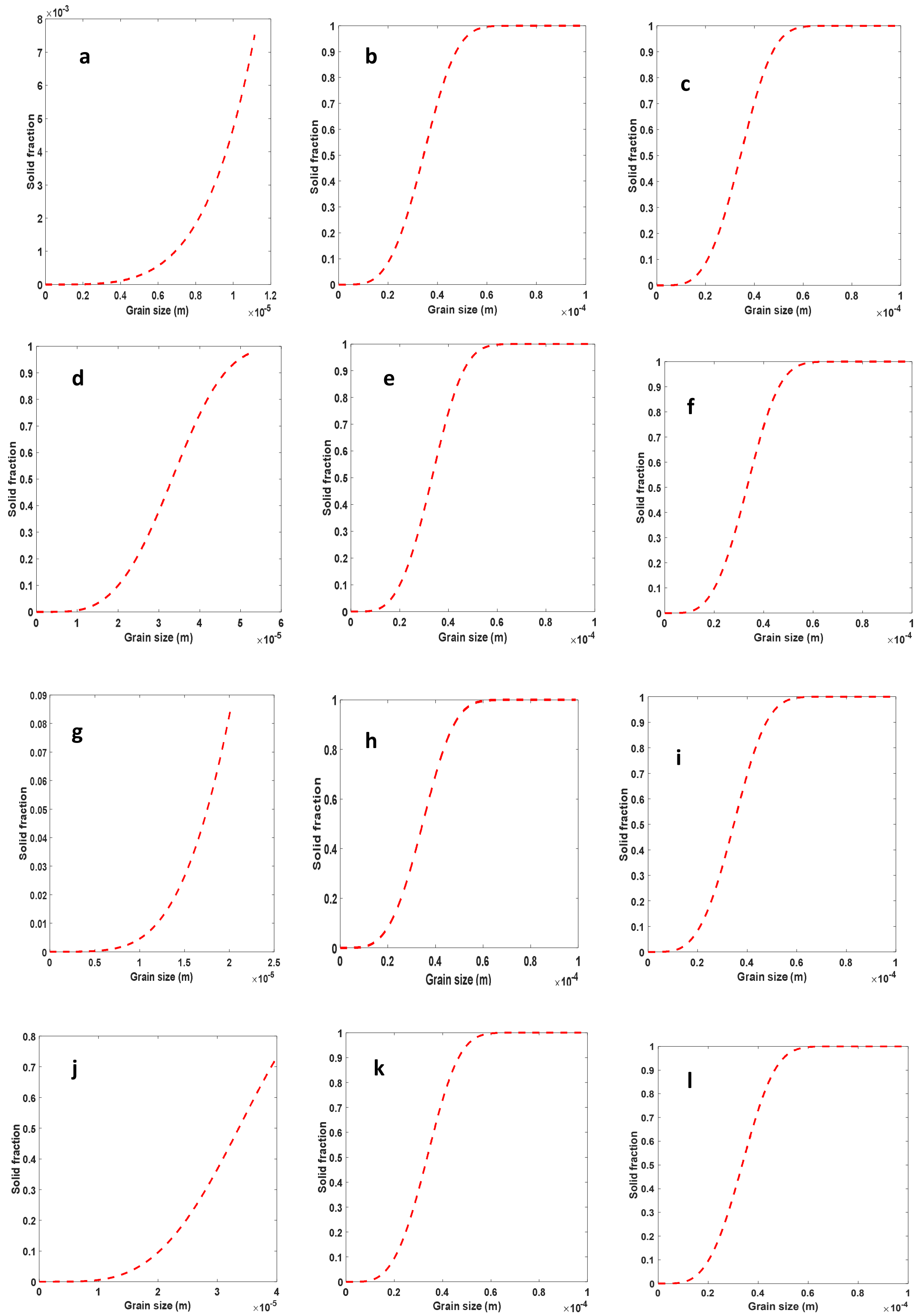

Fig. 9. Transient evolution of solid fraction and grain size for (a-c) Al-Cu (d-f) Al-Mg (g-i) Al-Si (j-l) Al-Zn eutectic alloys

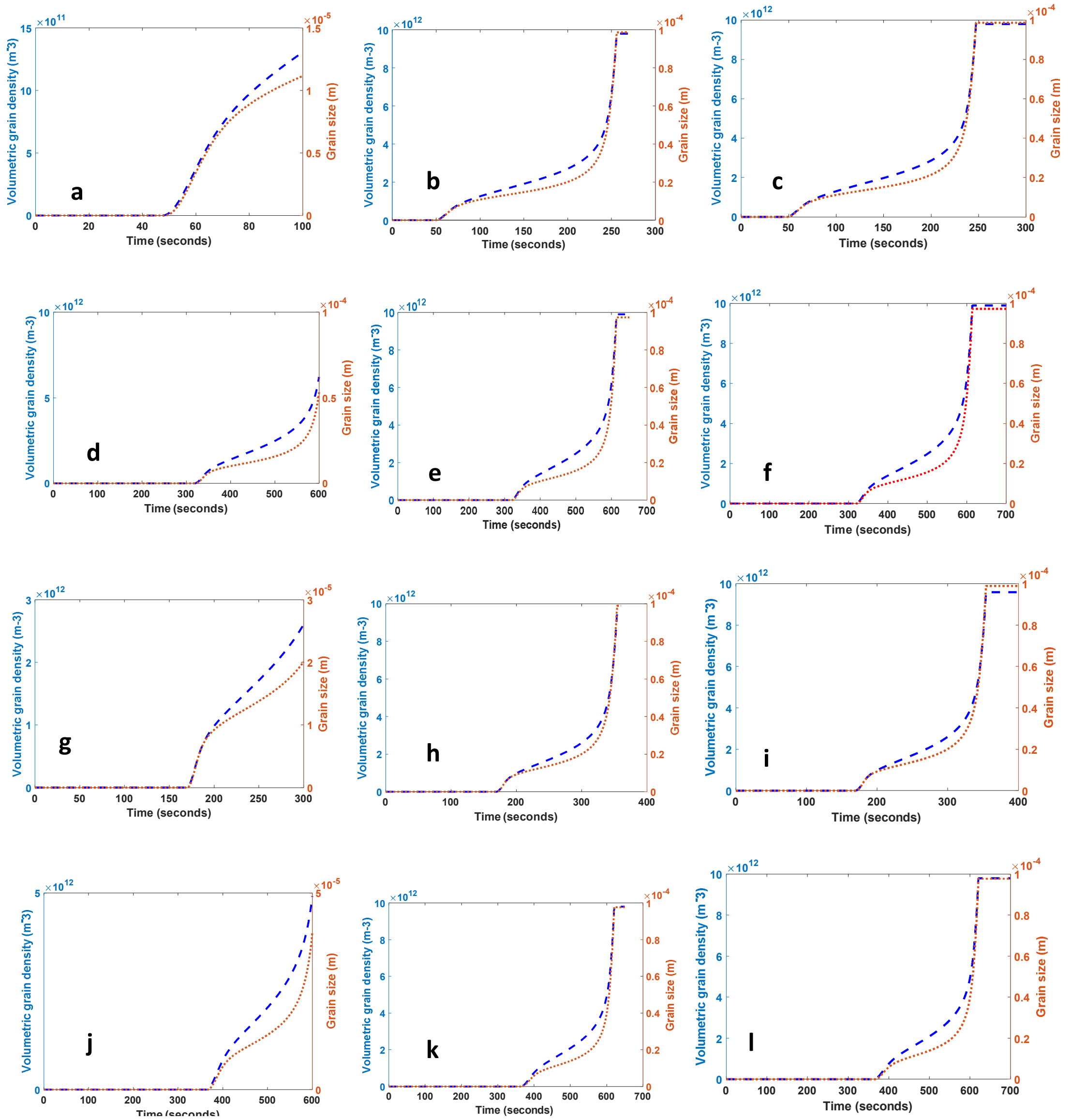

Fig. 10. Transient evolution of volumetric grain density and grain size for (a-c) Al-Cu (d-f) Al-Mg (g-i) Al-Si (j-l) Al-Zn eutectic alloys

4. CONCLUSION

The following conclusion can be deduced from the current study:

1. Under similar melt-thermal conditions within the mould cavities, the experimental cooling curves for Al-Cu alloy produced using metallic, sand, quartz and POP moulds are qualitatively similar. However, these materials respond differently to the presence of the liquid metal and therefore rate of evolution of the latent heat varied significantly. The metallic mould had the fastest cooling rate while the POP mould has the poorest heat extraction rate. Similar scenario played out on their period of isothermal phase change region where the metallic mould has shortest isothermal period while POP produced the longest period of isothermal transformation.
2. The simulated cooling curves for the four eutectic alloys solidified inside sand mould showed that Al-Cu and Al-Si have the fastest transformations while Al-Mg and Al-Zn have the slowest rate of cooling. The isotherms of Al-Mg and Al-Zn are longer than those of Al-Cu and Al-Si.

3. Mould size has significant influence on thermal distribution during solidification of eutectic alloys in static casting process as temperature tends to reach steady-state and homogenize faster in smaller moulds than bigger ones.
4. For all the alloys compared, nucleation period ranged between 25-50 seconds which is very small relative to the total solidification time. The better the thermal conductivity of the alloy, the narrower is the nucleation period and the greater the tendency for instantaneous nucleation.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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