A numerical study of the influence of pouring technique on the as-cast structure of Al-Cu ingots

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Abstract. Experimental evidence [Ohno 1987] revealed the influence of some pouring techniques on the as-cast structure. In the current work the process of pouring of the molten Al-4.0 wt.%Cu via one or multiple streams into a graphite mold is studied using a 3-phase model by considering the nucleation, the initial growth and transport of globular equiaxed crystals. The three phases are the melt, air and globular equiaxed crystals. Results showed that pouring via multiple streams increases the volume fraction and number density of crystals in the as-filled state. The subsequent solidification is calculated using a 5-phase mixed columnar-equiaxed solidification model. The five phases are the extradendritic melt, the solid dendrite and interdendritic melt inside the equiaxed grains, the solid dendrite and interdendritic melt inside the columnar grains. As final result the as-cast structure including the distinct columnar and equiaxed zones, columnar-to-equiaxed transition (CET), grain size, macrosegregation, and rest eutectic is predicted. Effect of melt convection and crystal sedimentation during the pouring and solidification is taken into account. The predicted as-cast structure, under the influence of single/multiple jet pouring, is evaluated by comparison with the available experiments of Ohno.

Introduction

The importance of pouring process in the formation of as-cast structure has since long been verified in the casting practice and in some laboratory experiments [1]-[6]. In addition to the melt treatment, parameters like the initial melt and mold temperatures, pouring rate, and pouring technique are mostly used by foundrymen to control the as-cast structure. However, the dependency of the as-cast structure on the above parameters is far from being understood.

One big challenge is the origin of the equiaxed crystals. The pioneer in-situ observations of Jackson and Hunt [7] conducted on the transparent ammonium-chloride solution showed that equiaxed crystals are formed during pouring of the superheated melt in a cold mold cavity. The solid crystals are detached from the mold wall and driven by the flow stream to survive in a sufficiently undercooled region, or remelt if the mixture is hot enough. During convection fragmentation of crystals may occur and the fragments can act as substrates for newly growing crystals. Ohno [5] conducted later on several experiments on metallic alloys, which seems to reveal a correlation of the origin of the equiaxed crystals to the pouring process. The as-cast structure is strongly dependent on the pouring methods. For example, pouring of a slightly superheated (~18 K) Al-0.2%Cu in a mold at room-temperature via one central pouring jet provided a mixed structure with more columnar fraction as shown in Fig.1a. Pouring via a side jet refines the structure (Fig.1b), while the proportions of the columnar and equiaxed zones are not significantly changed. Using multiple jets

(6 inlets) introduced a fully fine equiaxed structure (Fig.1c). Ohno attributed that very briefly to the effect of the wave motion at the surface of the molten metal.
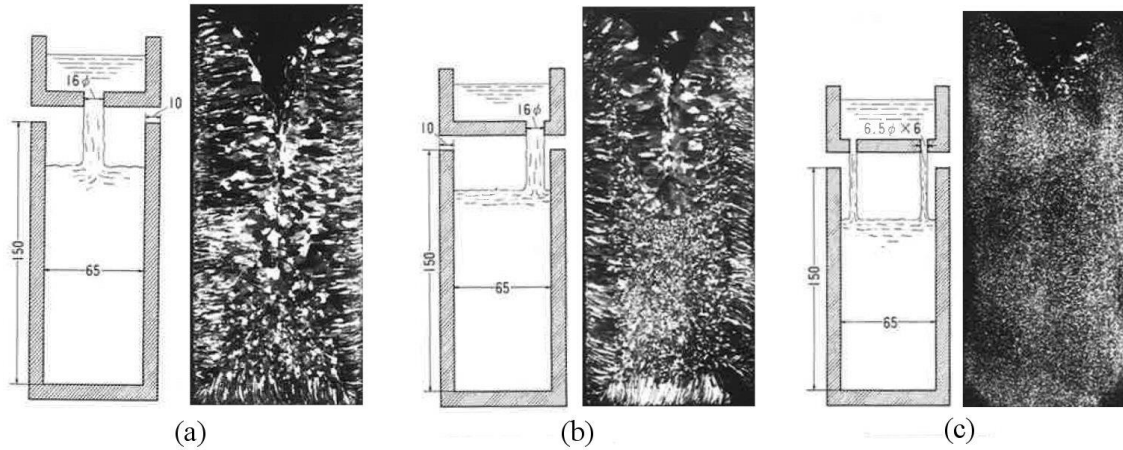

Fig.1. As-cast structures of Al-0.2%Cu poured at 953 K via (a) one central hole, (b) one side hole, and (c) 6 holes [5].

The lack of other experimental evidence and further theoretical study that support the interesting findings of Ohno motivated us to verify this phenomenon numerically. A 3-phase model was applied to simulate the mold filling. The results of filling were used as initial conditions for a 5-phase mixed columnar-equiaxed solidification model to calculate the formation of the as-cast structure. The Al-4.0%Cu alloy (poured at 1023 K) is used for the current study, since a set of consistent thermo-physical data and modeling parameters are available in literature. The simulation results are discussed and evaluated in the context of Ohno's results.

The model and simulation settings

For simulation of mold filling a 3-phase model [8]-[10] is used. The 3-phases are: the air phase, the liquid melt, and the solidifying equiaxed crystals. They are quantified with corresponding volume fractions, f_a, f_ℓ and f_e and they move with corresponding velocities, $\vec{u}_a$, $\vec{u}_\ell$ and $\vec{u}_e$. The liquid/solid mass exchange is calculated according to a diffusion-governed growth law. The air has no mass or species exchange with the other phases. The mass exchange introduces an additional source term for the momentum equation. The latent heat released during solidification is taken into account as a source term of the energy equation. A heterogeneous nucleation law [11][12] with three-parameter obtained from experiments [13] is used to calculate the nucleation of the equiaxed crystals, and it is considered as a source term for the transport equation of the equiaxed crystals. The melt is assumed to carry initially 10^{+7} m^{-3} of the heterogeneous nucleation sites.

The 5-phase mixed columnar-equiaxed solidification model is used to predict the as-cast structure and comprises three hydrodynamic phases: liquid melt, equiaxed crystals, and the columnar crystals, with corresponding volume fraction of f_ℓ, f_e, and f_c. They move with corresponding velocities of $\vec{u}_\ell$, $\vec{u}_e$, and $\vec{u}_c$ Here $\vec{u}_c$ is predefined (zero in the case of ingot casting), while $\vec{u}_e$ and $\vec{u}_\ell$ are solved numerically. The dendritic growth of crystals is taken into account. Two additional phase regions exist within the crystal envelope: the solid dendrites and interdendritic melt. Therefore, five 'thermodynamic' phase regions are defined in the system: the solid dendrites and interdendritic melt in the equiaxed grain, the solid dendrites and interdendritic melt in the columnar dendrite trunk, and the extradendritic melt. Each region has correspondingly volume fractions: f_s^e, f_d^e, f_s^c, f_d^c, f_ℓ, and characterized by its corresponding solute concentration: c_s^e, c_d^e, c_s^c, c_d^c, c_ℓ. Both hard blocking [14] and soft blocking [15] mechanisms are implemented and

applied to model the CET. For more details about the 5-phase model refer to previous publications [16]-[19].

For the mold filling, 3 different layouts of the pouring jet are configured, as shown in Fig.2: single central pouring jet, dual pouring jet, and a quadruple pouring jet. The pouring velocity and inlet area of single jet are estimated from experiments. Ohno's pouring process resembles a drainage problem of an atmospheric tank through an orifice with different diameters. Analogously, the total area of pouring jets is preserved. The diameter-dependent flow discharge coefficient is estimated for each case and the average pouring velocities are correspondingly calculated. The estimated filling times are 5.2, 5.77, and 6.1 s respectively. 3D simulation grids were constructed with ~ 85000 volume elements and an average grid size of 2.1 mm. For more details about the boundary conditions refer to [20].
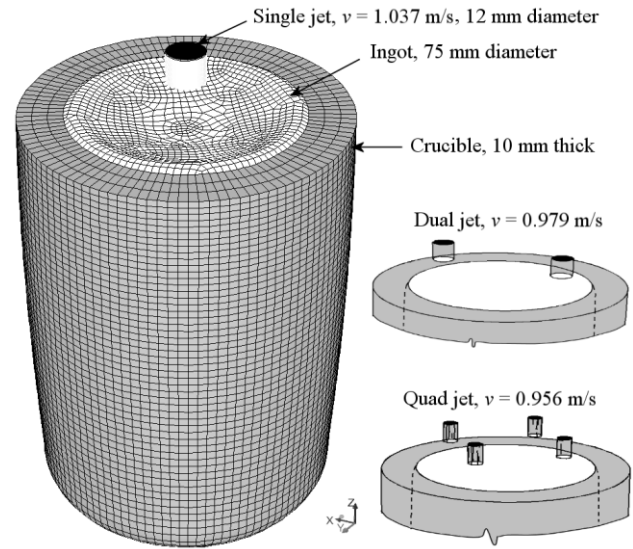

Fig.2. Simulation grid for mold filling and schematic of pouring method.

The average f_e and f_ℓ, grain number density of equiaxed crystals (n), and mold and ingot temperatures of the as-filled state are used to initialize the solution of the 5-phase simulation of ingot solidification. To reduce the calculation time, the problem is reduced to a 2D-axisymmetric with average grid size similar to that of the 3D/3-phase case. The development in temperature, phase fractions, and other quantities were recorded. During filling and solidification a fine time step of 10^{-4} -10^{-5} s was necessary to get a converged solution. Solidification time of ingot was ~470 s.

Results and discussion

During mold filling, premature solidification occurs when the superheat is low enough [20]. A preliminary numerical study of the influence of pouring technique on the mold filling, ignoring the discharge coefficient of the inlet, proved that pouring method has a trivial effect on n and f_e. Therefore, for the further calculations the flow condition at the inlet was slightly modified by considering the effect of the discharge coefficient on the pouring rate. The velocity per jet decreases by the reduction of the inlet diameter, i.e. the pouring rate decreases and filling time becomes longer accordingly. As shown in Fig.3, the higher the number of jets, the more quiescent is the flow. This is seen from the liquid/air interface for the 4-jet case (much less disturbances). Thus, it is expected for multiple-jet cases that n and f_e of the prematurely solidified crystals increase as a result of increasing the filling time and melt undercooling. The bottom of ingot exhibits lower temperature compared to the top (Fig.3a). Consequently, f_e and n are higher at the bottom (Fig.3b and c). The regions highly undercooled in Fig.3a correspond to the maximum f_e in Fig.3b and n in Fig.3c. By decreasing the number of pouring jets the velocity and the kinetic energy per jet increases and the flow tends to be more agitating, which carries the formed crystals away from the bottom as shown in Fig.4 and Fig.5a. The falling jet persists its superheat till it hits the bottom. Thus, the jet and the heat affected zone of the jet contains almost not crystals, whereas nucleation of crystals occurs at the supercooled ingot peripherals as shown in Fig.5b. Increasing number of jets reduces the kinetic energy per jet. Subsequently, the ability of jet stream to penetrate until the bottom to carry the formed crystals is reduced.
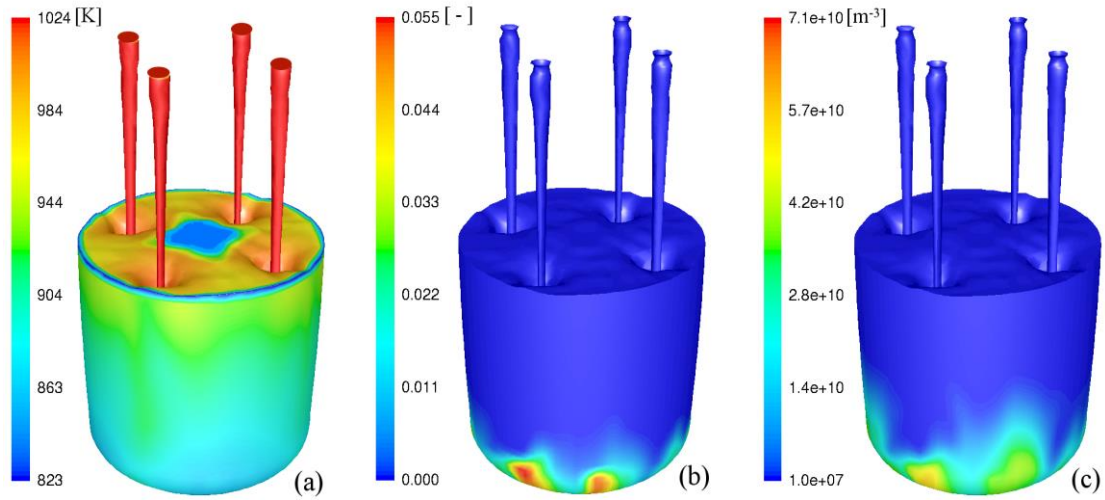
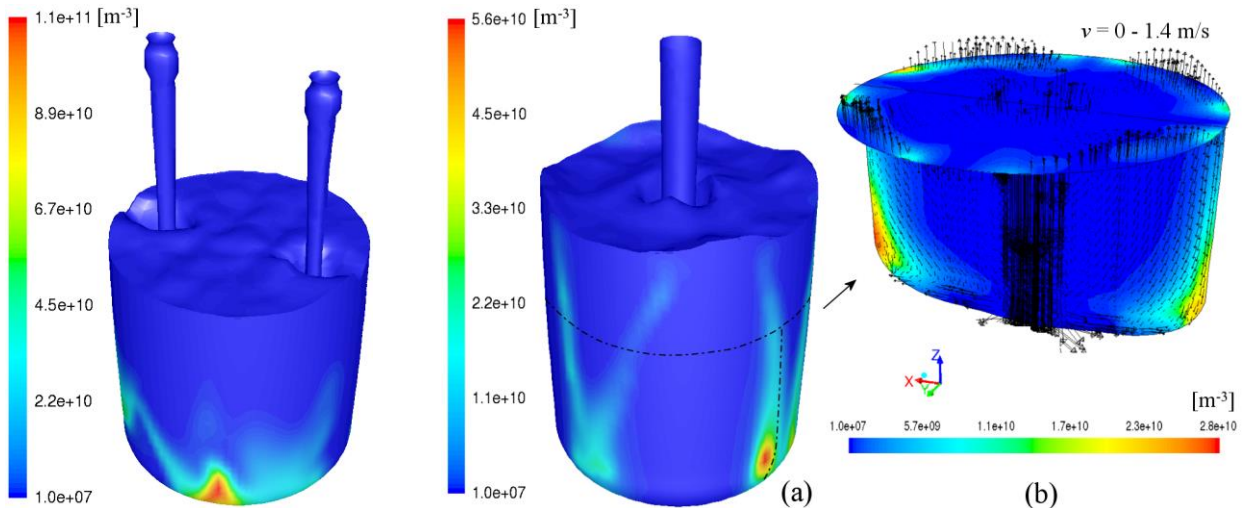**Fig.3.** Filling simulation results of the 4-jet ingot after 3.5 s for (a) temperature, (b) f_e, and (c) n.

Fig.4. The calculated n of the 2-jet ingot after 3.5 s.

Fig.5. The calculated results of the 4-jet ingot after 3.5 s of (a) n and (b) a cut as marked in (a) with a superimposed velocity of the liquid melt.

The development of the average n and f_e over the filled domain is shown in Fig.6. Nucleation starts for the multiple jet ingots at ~0.2 s when the melt hits the mold bottom. The number density drops after that due to continual pouring of the superheated melt. Nucleation rate increases again after ~1.4 s. Similar scenario is obtained for the single-jet poured ingot except that nucleation is delayed and the sudden n-jump disappeared because the pouring jet was faster and the initial contact area was more confined. Solid fraction increases gradually with time. The higher the number of pouring jets the higher the solidification rate and higher the average f_e.
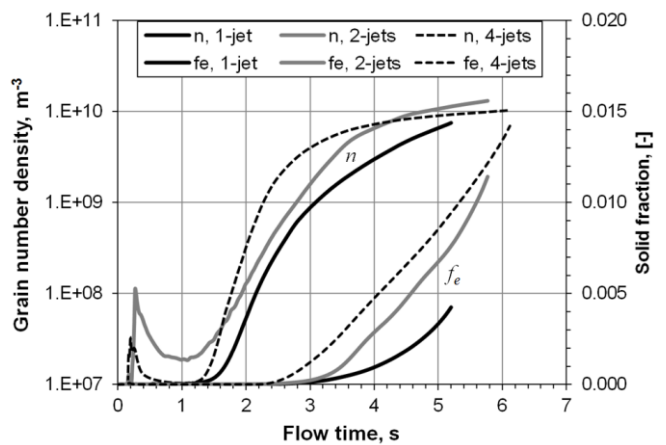

Fig.6. Development of the average n and f_e over the filled domain.

The results of the ingots at the as-filled state are used as initial conditions for the 5-phase simulations. The distribution of phase fraction for the ingot poured via 4 jets is shown in Fig.7a and b. The ingot top exhibited higher f_c, whereas the structure at the lower part is almost equiaxed. The number density of equiaxed grains (Fig.7c) is high at the ingot core. Sedimentation of the equiaxed crystals during solidification increases n close to the bottom. The macrosegregation map is shown in Fig.7d. Negative macrosegregation is predicted in the equiaxed region, while positive macrosegregation is obtained at the mixed columnar/equiaxed zone above the CET line. Macrosegregation is analyzed by the mixture concentration c_{mix}, being calculated according to the volume fraction of rest eutectic and solid within the equiaxed and columnar grain envelope. The final distribution of the phases is the outcome of the melt flow and crystal sedimentation. The phase distribution of the ingots poured via 2 jets (Fig.8a) or 1 jet (Fig.8b) is qualitatively similar to that shown in Fig.7a. The quantity of the average f_e is also not significantly changed. The average f_e over the whole casting domain lies in the range of 0.67-0.70.
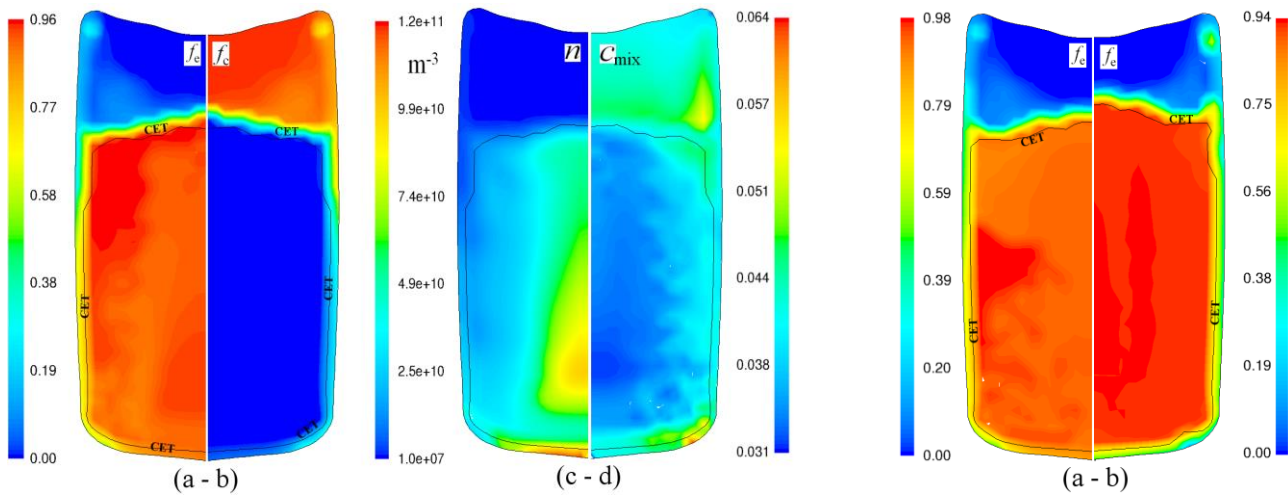

Fig.7. Predicted as-cast structures of the 4-jet poured ingot of (a) f_e, (b) f_c, (c) n [m^{-3}], and (d) c_{mix} [-].

Fig.8. Predicted f_e for the (a) 2-jet and (b) 1-jet poured ingots.

The mold filling results show that increasing the number of pouring jets, keeping the total inlet area, increases filling time and affects the melt/mold interaction. Correspondingly, the volume fraction of the prematurely solidified equiaxed crystals formed during filling increases as well. An average f_e of 0.01411 is obtained for the 4-jet filled ingot compared to 0.0043 obtained for the single jet case. Thus, the variation of ~0.01 seems to be insignificant for the initial conditions of the 5-phase simulation as shown in Fig.7a and Fig.8b. In addition, the reduced 5-phase model sensitivity to the initial conditions can be attributed to using averaged values. Interpolating the distribution of the solidification quantities of flow, temperature, and phase fraction fields from the filling simulations to initialize the solution of the 5-phase model led to an unavoidable solution divergence. Furthermore, the filling is solved here as a 3D problem, whereas the as-cast structure is solved in 2D and axisymmetric. This is expected to influence the solution accuracy. Using 3D-grid to conduct 5-phase simulation is too costly. Such drawbacks will be taken into consideration in the future works. However, the current 5-phase model have been proved a good agreement with the experiments in previous works [20][21].

On the other hand, some important information of Ohno's experiment (Fig.1) is missing. In the experiment, the inlet area and the metal head within tundish were maintained, whereas the influence of discharge coefficient on hydrostatic head losses and the filling time were not discussed. The low superheat of the poured melt (18 K) makes the experiment very sensitive to temperature variations. In the simulation the inlet temperature is so simple to control but in practice the melt temperature in the pouring tundish is locally and chronically changing. Previous investigations [20] showed that melt superheat is a key parameter for the as-cast structure. Ohno did not sufficiently argue, why

using 6 pouring jets in filling introduced a fine fully equiaxed structure as shown in Fig.1c. This structure has just been attributed to the wave motion of the melt that concentrate around the surface of the molten metal [5]. The lack of similar experimental studies invokes the researchers to verify Ohno's results.

Conclusion

The mold filling simulation with a 3-phase model has succeeded to respond to the minor flow variation due to multiple-jet pouring. The domain averaged as-filled result over the ingot section is used as initial condition for the subsequent solidification calculation with a 5-phase model. The fraction of the prematurely solidified crystals at the as-filled state is predicted to increase with the number of pouring jets. The as-cast structure is, however, predicted to be less sensitive to the number of pouring jets. It seems not to agree with the Ohno's experiment. We suggest that the as-filled flow field, which was currently ignored, should be considered as a part of initial condition for the subsequent solidification calculation in future. Additionally, verification of Ohno's results is necessary in the outlook.

Acknowledgment

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