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Simulation of the Extensional Flow Mixing of Molten Aluminium and Fly Ash Nanoparticles

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Abstract**—**This study presents simulations of an aluminium melt containing an initially non-dispersed fly ash nanoparticle phase. Mixing is affected predominantly by means of forced extensional flow via either straight or slanted orifices. The sensitivity to various process parameters is determined. The simulated process is used for the production of cast fly ash-aluminium nanocomposites. The possibilities for rod and plate stock grading in the context of a continuous casting process implementation are discussed.

Keywords**—**Metal matrix composites, fly ash nanoparticles, aluminium 2024, agglomeration.

I. Introduction

FOR the production of cast fly ash-aluminium nanocomposites it is necessary to achieve good dispersion of the fly ash nanoparticles (NPs) inside the molten aluminium matrix. Stirring by means of an impeller and sonication are two popular methods for achieving this. Direct use of positive-displacement-forced extensional flow is also a possibility, i.e. by use of a pulsating perforated piston, based on prior experience with mixing plastic matrix-CNT composites. While all three methods have been verified in various studies to achieve the intended mixing results, there is no common benchmark established on their relative effectiveness, i.e. in terms of mixing efficiency (time, energy) and uniformity of dispersion.

Metal matrix composites (MMCs) reinforced with NPs have been extensively studied and widely used in the aerospace, automotive, and military industries due to their high strength-to-weight ratios and enhanced mechanical and thermal properties including specific modulus, superior strength, stiffness, good wear resistance, fatigue resistance and improved thermal stability [1]-[4]. There has been an increasing interest in composites containing low density and low cost reinforcements. Among the various reinforcements used, fly ash is one of the most inexpensive and low density reinforcements available in large quantities as solid waste by product from combustion of coal in thermal power plants [5], [6], and fly ash particles are collected from electrostatic precipitator. This waste has been suggested to be suitable for use as reinforcing materials in MMCs [7], [8]. A number of researchers have been studied on the influence of fly ash on the mechanical properties of MMCs. Rohatgi et al. have found slight improvement in hardness, tensile properties, and wear resistance of fly ash reinforced AZ91D based composites [9]. Gikunoo et al. reported that reinforcing materials with fly ash in cast alloy A535 based composites reduced the tensile strength and hardness of the composites due to segregation and particle clustering of the fly ash in the aluminium matrix [10]. Anilkumar et al. suggested that the tensile strength [7], compressive strength, and hardness can be increased by increasing weight fraction of fly ash up to 15% in Al (6061) based composites, also they obtained uniform distribution of fly ash particles while increasing weight fraction of fly ash. A reduction in particle size of fly ash increases the strength (tensile and compressive) and hardness of the resulting composites. Murthy et al. have been achieved a reduction in particle size of fly ash from micrometer level to nanometer levels by using a high-energy planetary ball mill [6]. In their results, the nanosized fly ash addition leads to improvement in the compression strength of the composites. Moreover, low density and low cost are other attractive benefits of fly ash [10].

However, it is extremely difficult to achieve uniform dispersion of nanosized fly ash particles in liquid metals due to high viscosity, poor wettability in the metal matrix, and a large surface-to-volume ratio, which results in agglomeration and clustering [4], [11]. So far, several fabrication technologies of producing MMCs have been developed such ash including high-energy ball milling [12], in situ synthesis [13], electroplating [14], and ultrasonic stir casting technique [11], [15], [16]. Previous studies have shown that, among these techniques, ultrasonic stir casting technique is a promising method to fabricate the nanosized particle-reinforced MMCs. Also, this technique is supposed to be more reliable and cost effective.

In this study, multiphase two-dimensional CFD simulations are conducted for an aluminium melt containing an initially poorly dispersed fly ash NP phase, which is subjected to mixing via a forced passage through consecutive straight and slanted orifices. In this layout, extensional flow mixing becomes dominant. The flow mechanisms leading to the eventual fly ash particle dispersion are observed and compared. In order to investigate forces causing the agglomeration of fly ash NPs in molten alloy and the conditions favouring breaking up of these agglomerations, a

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numerical model is needed. By a numerical model, the behavior of the cluster of NPs under various conditions can be simulated. In this study, an ANSYS FLUENT Eulerian Granular Multiphase Model (EGMM) was adapted. The numerical EGMM accounts for turbulent fluid flow, volume fraction, and the complex interaction between the molten alloy and NPs. Geometry of mechanical mixing chamber, volume fraction of fly ash NPs, and other parameters dependence on dispersion NPs in molten alloy were investigated.

II. Model

Fig. 1 shows schematic illustration of an original custom-designed stir-casting equipment considered for numerical simulation. Normally, the design features a filter undergoing a reciprocating motion inside a cylindrical cavity that is containing the melt. As a first step to the process, the Al alloy powder and fly ash NPs are mixed and inserted into the mixing chamber. The mixing process starts after maintaining the temperature at the required melting point. The movable filter moves horizontally in the mixing chamber by electrical motor, and once movable filter comes to the edge of chamber, then it returns back. Thus, the filter continuously repeats the motion in the chamber, and molten alloy passes through by holes on the filter, respectively. This mechanical mixing process is expected to dramatically improve the uniform dispersion of nanosized fly ash particles in the melt. The moving frequency, melting temperature, geometry of filter, volume fraction of fly ash particles can be tuned for getting to achieve uniform dispersion of particles in liquid alloy. However, in this study, we consider not a single but several such filters fixed at given positions along the cylindrical cavity and an external positive displacement pump forcing the melt to pass through the filters in a continuous constant velocity motion (single pass). This process requires a longer cavity, but is potentially more efficient, as it eliminates the requirement for a reciprocating motion, simplifies the design by reducing sealed interfaces, and lends itself better to an implementation featuring a continuous casting principle.

The geometry of the computational model (showing a single filter instance) is shown in Fig. 2. The corresponding mixing chamber segment has a diameter of 56 mm and length of 100 mm. The liquid phase is Al alloy 2024. It has a density of 2780 kg/m^3 and viscosity of 0.001 kg/(m.s). The fly ash NPs with an average particle size of 100 nm and density of 2250 kg/m^3 are treated as granular-particles. The Al alloy is considered as phase 1 and the fly ash as phase 2. The temperature of molten ally and fly ash particles is set to 770 °C. Mixed alloy and fly ash NPs were inserted into the chamber with a velocity of 2 m/s from inlet 1, and pure Al alloy was injected via inlet 2 at the same velocity.

The finite element mesh used is shown in Fig. 3. High smoothing and six inflation layers are used for simulation.

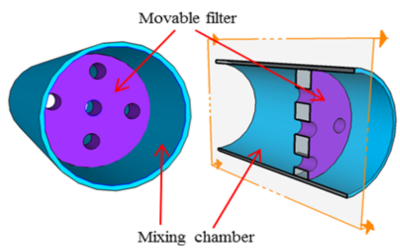

Fig. 1 Schematic view of Custom-designed stir-casting equipment considered for numerical simulation. In the present study, the filters remain fixed and the flow is induced by an external positive displacement pump

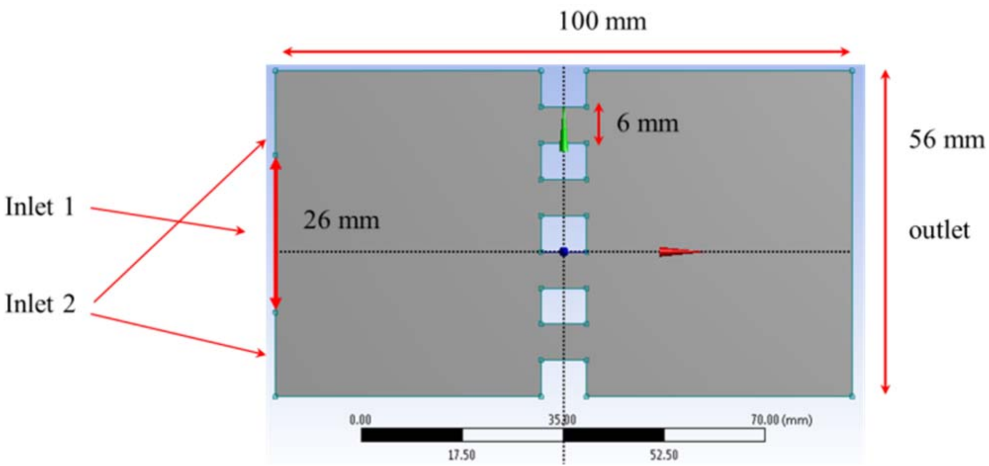

Fig. 2 Geometry of the computational model. The inhomogeneous inlet melt is simulated as a pair of two distinct homogeneous inlet melts with different volume fractions

Relevance center	fine
Smoothing	High
Curvature normal angle	18°
Minimum size	0.00001
Maximum size	0.0015
Maximum face size	0.001
Growth rate	1.2
Minimum edge length	0.002
Inflation maximum layers	6

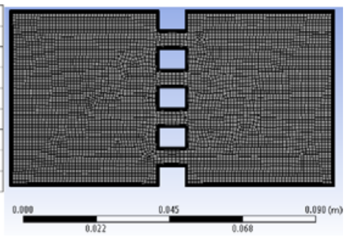

Fig. 3 Mesh details used for the simulation

III. Results and Discussion

A. Fly Ash NP Dispersion

Using the developed numerical model, the mixing process of Al alloy and fly ash NPs was simulated. Fig. 4 presents the velocity distribution in the mixing chamber at steady state. As expected, the filter holes act as choke points, creating the dominant effect of extensional flow mixing. Fig. 5 shows the turbulent kinetic energy, which is maximised after the exits of the filter holes. The fly ash volume fraction map is shown in Fig. 6, indicating the gradual dispersion of the fly ash throughout the melt after each filter pass. The degree of mixing is graded in the lateral direction. The obvious trend is that the mixture tends to retain the symmetry of the original inlet pattern; however, this is disturbed somewhat by the lateral offset that has been introduced between the successive filter hole patterns.

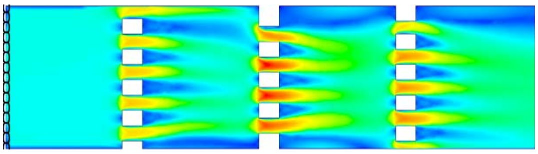

Fig. 4 Velocity (steady state)

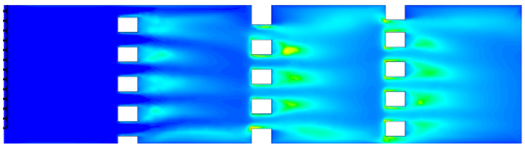

Fig. 5 Turbulent kinetic energy (steady state)

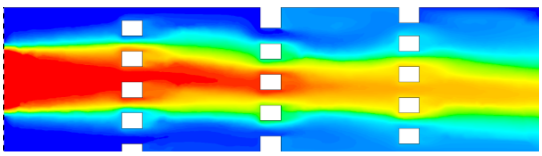

Fig. 6 Volume fraction fly ash (steady state)

B. Transient Analysis

A transient analysis of the same mixing problem was conducted, to assess the time required until steady state is reached and to provide more insights about the effect of filter placement on the mixing phenomena. The initial condition was that the cylindrical cavity was filled with Al alloy, with complete absence of fly ash. Fig. 7 shows the propagation of the 'disturbance' through the simulated volume as a fly ash volume fraction is introduced through the centre inlet, until a new steady state is reached.

C. Application to a Continuous Casting Process

Combining the insights from sections A and B, we observe that the studied layout provides some interesting possibilities if used in the context of a continuous casting process:

- The provision of two (concentric or otherwise) inlet zones allows for the cross-section-wise grading of the produced cylindrical rod/plate. In this case, fly ash was inserted via the middle inlet, but this may be reversed. Given well-documented improvement in the tribological properties of fly ash aluminium and the detrimental effect on toughness, this process can be used to produce soft-core hard skin rod and plate stock in a single casting stage, without need for surface treatment a posteriori.
- Variation with time of the feed rate of the fly-ash-rich phase compared to the Al alloy phase allows the length-wise (longitudinal) grading of the produced rod or plate stock. As the transient simulations show, any change in inlet composition tends to move, especially through the first few filters where the effect is sharper, as a propagating front. This can also be used to create various batch compositions in sequence without disrupting (stopping/restarting) the casting process and with minimal scrap/ out-of-spec material.
- The distance and lateral offset between the filters and the number of filters can be expected to significantly affect the mixing. Few filters separated by large distances and having zero lateral offset will result in minimal mixing, while several closely spaced and heavily offset filters will maximise it. This effect can be used creatively when any sort of material grading, as discussed previously, is desired. The effects of these parameters will be the object of a subsequent study.

D. Sensitivity Analysis

A sensitivity analysis was conducted considering the effect on mixing of particle size, melt temperature, inlet velocity, and fly ash volume fraction. Besides the obvious effect of the volume fraction, neither of the other factors seem to affect the simulated behaviours significantly, and the same trends were confirmed.

The effect of geometric parameters, such as the filter hole size and area ratio, the hole offset, the number of filters and the distance between the filters are expected to have a much more significant effect. This analysis will be reported in a subsequent study. In the following section, a preliminary study of the possible effect of tilting is presented.

E. Effect of Tilting of the Filter Geometry on the Fly Ash NP Dispersion

After investigating effects of volume fraction of fly ash NPs on the dispersion of the particles in molten alloy, the effect of tilting the filter orifice patterns was investigated. All modelling parameters were kept same as in the previous section, only geometry of filter holes of mixing chamber has changed (see Fig. 8).

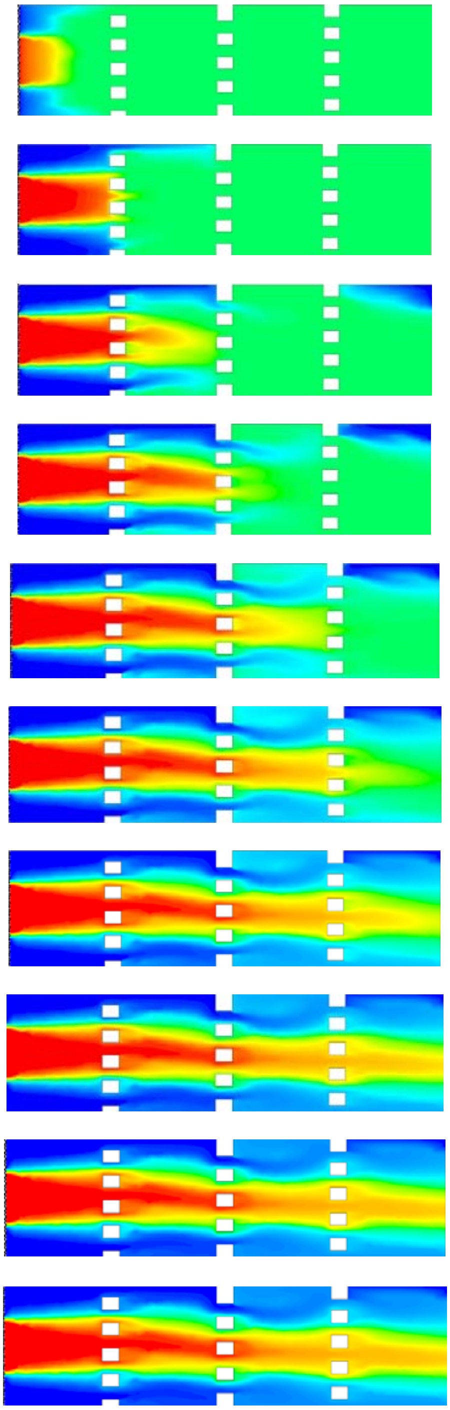

Fig. 7 Volume fraction fly ash (transient). Snapshots taken every 60 ms, showing steady state achieved after approx. 600 ms

The filter holes were tilted 26 degrees downward or upward, while their diameter and the length of filter are not changed. Figs. 9-11 show the calculated velocity, turbulent kinetic energy, and fly ash volume fraction maps at steady state. Although significant turbulence is seen, the flows from the two inlets remain relatively cohesive, and in fact, the mixing is somewhat poorer compared to Fig. 6. It is hypothesised that because the density of the fly ash particles is comparable to that of the Al alloy, the centrifugal effect imposed by the tilting does not cause additional dispersion. If a much heavier phase was involved, then the result could be quite different. As it stands, there does not seem to be a merit in using this tilting principle.

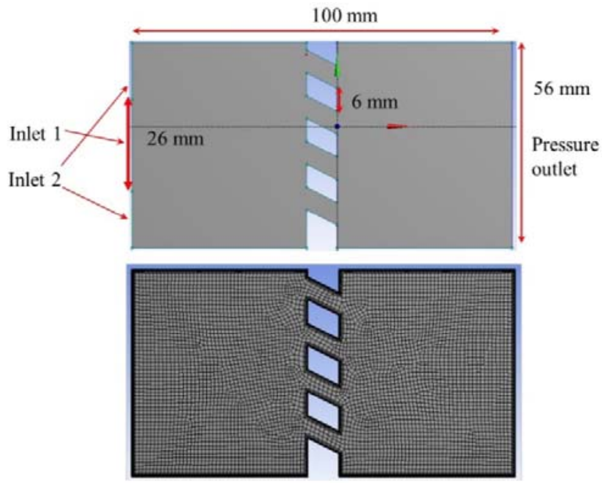

Fig. 8 Mesh details used for the simulation

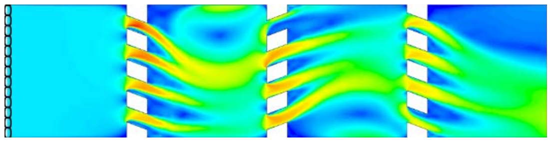

Fig. 9 Velocity (steady state)

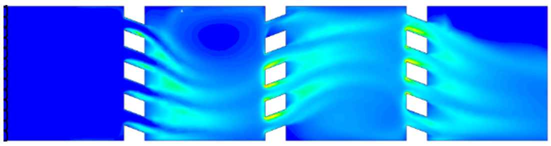

Fig. 10 Turbulent kinetic energy (steady state)

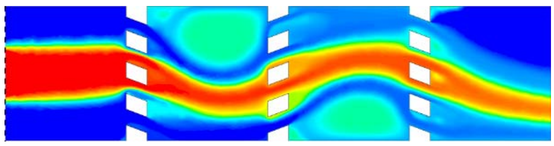

Fig. 11 Volume fraction fly ash (steady state)

IV. Conclusion

The ANSYS FLUENT numerical EGMM model is used to investigate the distribution of fly ash NPs into an Al 2024 matrix with different volume fraction and geometry of chamber filter under custom designed stir casting equipment. It was determined that a strong extensional flow, particularly by using subsequent filters with laterally offset hole patterns, can disperse the NPs relatively well. Also, it was demonstrated that the geometry of chamber filter, e.g. the angle of the hole patterns, can play a significant role in the dispersion during the mixing process.

The studied layout also showed potential in creating laterally and longitudinally graded rod and plate stock if used in the context of a continuous casting process.

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