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Sedimentation Of Inclusions In Melts Of Aerospace Structural Aluminium Alloy Castings: A Sustainable Approach

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Abstract

Achieving the full potential of mechanical- and other- properties in aerospace structural aluminium alloy castings is often hindered by the presence of detrimental inclusions in the melt during casting. The inclusions arise from high-temperature chemical reactions and the dissolution of substances in contact with the melt or pre-existing in the alloy. Suitable additions to the melt can precipitate on the inclusions and cause them to sediment, resulting in cleaner melt.

Simulation techniques were employed with commercial software packages (Flow3D) using high performance cluster computing (HPC) facilities to analyse the behaviour of impurity particles of various sizes and distributions under different boundary conditions such as temperature, pressure, flow rate, and heat transfer. The simulations provide insights into the sedimentation process to identify effective methods for eliminating/reducing these particles from the melt. Some of the practical melt-holding or processing challenges, and mitigations, are also discussed.

Keywords: **Aluminium alloys, impurity elements, sedimentation, simulation, sustainability, aerospace castings, HPC.**

Introduction

Approximately, 1.5 million people are residing in the sky, flying at any time. That is more than 10000 aircraft consuming carbon emitting fuel. At least a total mass of approximately 1.3 Gg is in the sky in the form of human and human made objects. Humanity's increased demand for air travel is causing rapidly increasing direct- and indirect- emission that needs attention for a sustainable future.

Aluminium is regarded as a permanent metal that could be recycled indefinitely though not

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without inevitable challenges. The metal is prone to react with the atmosphere during casting, producing a surface oxide film which can be entrained in the metal folded over to constitute a crack known as a bi-film [1]. Recycled aluminium alloys can have dense populations of bifilms which reduce properties, especially ductility, toughness and fatigue. The entrained oxide films are not only detrimental to its mechanical properties but, if in sufficient quantity, can also keep up on the surface of the liquid, causing economic loss as dross. Other impurities in solution, notably iron, can build up during recycling to further degrade properties. The special focus was on the sedimentation of alumina (bi-film) or non-dissolved inclusions whereas dissolved detrimental elemental removal may be a supplement of this simulation or future work.

Aerospace applications have been attracted to aluminium alloy due to its good specific strength, as indicated by the purple arrow and circle in the Figure 1, that could be improved further through proper melt treatment before casting. The current market is demanding greener aviation. The UltraCleanCAST project is focusing on addressing this issue through sedimentation techniques to achieve melt cleanness. As part of the project, the simulation techniques have been implemented to support the practical trials at a manufacturer who is part of this project.

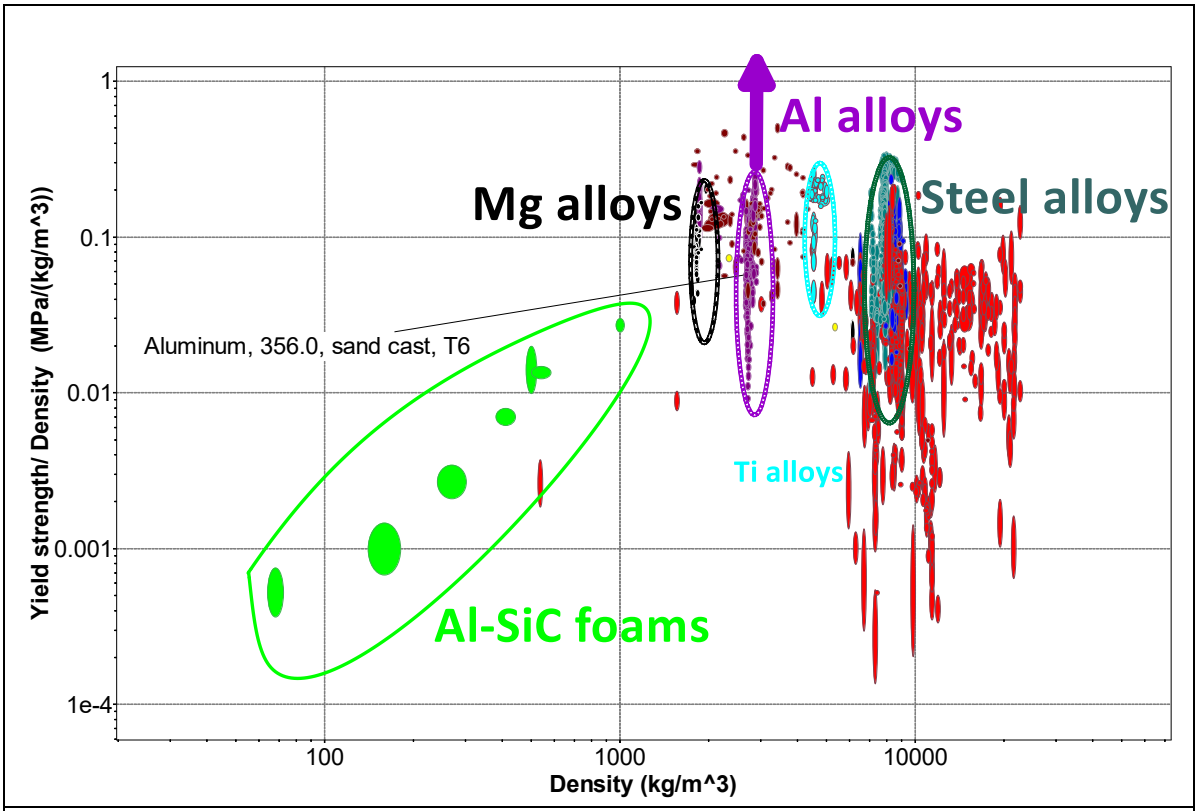


Figure 1: The specific strength (yield strength/density) of potential or currently utilized aerospace materials as a function of their density indicates that aluminium alloys could be the preferred candidate for sustainable aviation if their potential specific strength can be fully realised. The chart was generated using the widely recognized Ansys Granta EduPack, [2] , drawing from its comprehensive materials property library.

Al-Si alloys are widely used in the aerospace applications due to their favourable properties such as high specific strength, castability, and abundance of these elements. However, the presence of inclusions such as alumina bifilms, dross, and other non-metallic inclusions or any

detrimental intermetallic particles formation during the casting process can significantly affect the mechanical properties of these alloys. Understanding and controlling sedimentation of these inclusions by simulating these processes, are crucial steps in improving melt cleanness and achieving superior mechanical properties in Al-Si alloys, especially the A356 and A357 alloys.

Alumina bifilms are among the most prolific and injurious inclusions introduced during the turbulent pouring of the melt, but interestingly, also act as nucleation sites for intermetallic phases. This behaviour is utilised as a mechanism for the elimination of the bifilm cracks by arranging for elements in solution in the alloy to precipitate as intermetallic compounds on the bifilms. The weight of the intermetallics causes the bifilms to sink, freeing the melt from its population of cracks.

Cover flux, typically composed of NaCl, KCl, and $MgCl_2$, is used to minimize oxidation in aluminium alloys, either alone or in combination with a controlled atmosphere of inert gases. In addition to minimizing oxidation, fluxes serve other important functions such as drying dross by wetting the Al-melt and aluminium oxide (typically with NaCl-KCl and additives like CaF_2 or Na_3AlF_6), reducing alkali and alkaline-earth elements such as Na, Ca, K, and Li (using eutectic blends of KCl and $MgCl_2$), and facilitating furnace cleaning through the use of exothermic salts. Titanium is generally added for grain refinement, often in the form of an Al-Ti master alloy or Al-Ti-B rod. Titanium powder is typically not added directly in aluminium casting processes due to its high reactivity at elevated temperatures, which poses significant risks and potential complications in the melt. The scope of this paper is to simulate the sedimentation process of bi-films (primarily), which are typically sheet-like structures and cannot be treated as conventional particles. However, recent findings by, Gyarmati et al. [3] suggest that the controlled precipitation of intermetallic phases, such as $(Al,Si)_3Ti$, on bi-films can alter their behaviour, causing the bi-films to behave more like particle inclusions. This interaction facilitates their sedimentation and removal from the melt, contributing to a cleaner melt and improved casting quality, as depicted in Figure 2. Therefore, while the focus remains on the bi-film's sedimentation process, the formation of intermetallic phases on bi-films introduces an additional factor that can influence this process. The combined structure of the bifilms and the $(Al,Si)_3Ti$ crystals that nucleate on them exhibit intricate shapes. However, for simplicity and due to limitations of the simulation platform, these are modelled as crystalline shapes. The drag coefficients for different shapes (such as sheets, cylinders, pyramids, cubes, etc.) could be adjusted to yield more realistic simulation outcomes. Henceforth[1], the term "inclusions" or "particles" refers to these complex shapes (the combination of bi-films and $(Al,Si)_3Ti$ crystals).

[11] Unless specified as different particle.

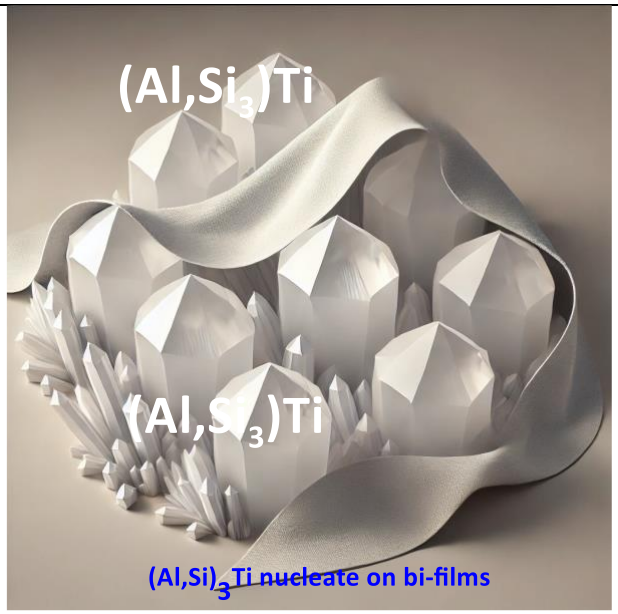


Figure 2: An illustration shows how pre-existing alumina bifilms act as nucleation sites for $(Al,Si)_3Ti$ crystals with faceted morphology, allowing them to grow and eventually sediment within the launder system. Nucleation occurs on bifilms when the solute becomes supersaturated, and once an atomic-sized particle forms, the $(Al,Si)_3Ti$ crystals grow through solute diffusion. The increasing particle size and higher density compared to the melt lead to rapid sedimentation, is affected by convective flow; the movement of the liquid may help or hinder the sedimentation process.

Zhang et al [4] demonstrated that with a 0.06 T magnetic field effectively improved sedimentation of alumina particles in an aluminium melt of commercial purity; 30 µm particles took a few seconds to settle in their mould. Although, this would seem to be attractive for pure aluminium, for multi component Al alloys the effect of magnetic field is complex and maybe detrimental or cause segregation of alloying elements and hence sediment all non-metallic inclusions together with the alumina particles.

Szucki1 et al. [5] studied the particle behaviours, using Flow3D software, within a mould filling process that targeted the solid inclusions within the melt. They used (10 and 100) µm particles with densities of (1350, 2700, and 5400) kg/m^3. Due to the solidification beginning at the mould walls, inclusions are typically trapped around the outer layers of the casting. However, the final distribution of inclusions is influenced by multiple factors, such as the mould filling process, the relative densities of the particles and the melt, and the cooling rate. Szucki1 et al. [5] conducted a numerical analysis of solid particles flow in liquid metal during casting, highlighting how such factors play a critical role in particle transportation. Thus, it is crucial to eliminate these inclusions from the melt prior to casting. While convective heat flow is complex and can significantly influence heat transfer (within the launder or out of the launder), the cooling rate in our system is not actively controlled, as the launder primarily serves for melt transport. Nevertheless, unintentional heat loss may occur during the process, which can impact the solidification dynamics and cause inclusions to be transported to the solidification front, potentially accumulating in the lower basin of the launder. Therefore, this sedimentation can be removed periodically.

Another study [6] on the segregation behaviour of Mg_2Si particles (density 1990 kg/m^3), using ANSYS Fluent software, during centrifugal casting showed the particle distribution could be controlled by the rotational speed or segregated as a function of this speed, hence a functionally graded material could be manufactured. During centrifugal casting, the molten metal is subject to strong centrifugal forces, which act on both the molten phase and any precipitating particles, including Mg_2Si. Even though Mg_2Si precipitates later in the solidification process, it still exists as a separate phase within the molten metal for some time before being fully trapped by the solidifying aluminium matrix. The centrifugal force can drive these precipitating particles toward the inner wall of the casting (because they have a lower density than aluminium), allowing some level of segregation before the solidification front completely encloses them. The study using ANSYS Fluent demonstrated that, despite Mg_2Si precipitating later, segregation was still possible due to the interactions between the buoyancy and centrifugal forces acting on the particles during the casting process. Even with solidification underway, the remaining molten phase allows Mg_2Si to move under the influence of these forces until it is finally "frozen" into the solidified structure.

In summary, attempts to separate the non-metallic unwanted inclusions from multi-component or pure aluminium melt, such as gravity sedimentation, flotation, flux refinement and filtration, as well as magnetic field application, have never achieved industrial application. However, other than the above referenced studies there could not be found any open literature that focused on particle sedimentation in Al-Si alloys using computer simulations in order to precipitate them before casting, especially the detrimental bifilm of alumina in A356 or A357 alloys for aerospace structural applications. The growing market for greener manufacturing requires processes which are simple and economical. Therefore, the UltraCleanCAST project adopted flux to protect the melt while the cleanness of Al-Si alloy melts was improved through controlled sedimentation of inclusions. Enhanced melt handling can significantly improve the mechanical properties of castings. The sedimentation process is expected to be encouraged by the suppression of convection within a newly designed launder system. Computer simulations play a vital role in predicting the behaviour- and the effects- of the inclusions during- and after-melt handling and optimising processing parameters to achieve better performance of these alloys in aerospace applications for a sustainable future to promote responsible consumption of limited materials. The particle sedimentation simulation with high performance computer has been the focus of this study.

Methodology

The project involves a combination of simulations and practical trials. The simulations are conducted using Flow3D software at Cranfield University's high performance computer facility (The Delta2 HPC systems). Practical trials are performed at Sylatech's facilities.

The following steps were implemented,

-Defining boundary conditions based on physical measurements.
-Modelling various particle sizes and densities.
-Analysing the effectiveness of particle sedimentation.
- Iteratively optimizing the launder system design and or processing parameters/initial – and boundary- conditions where possible.

Simulation and Practical Trials

The project involves both simulation and practical trials for a launder system, a cleaner melt delivery system for rapid casting production. The practical trials are carried out at our industry partner Sylatech's facilities, while Cranfield University supports the project with simulations using its HPC systems. The simulation with Flow3D software incorporates particles to represent Al_2O_3 (the bifilm)), onto which Fe and other heavy elements in solution can precipitate in the form of intermetallic and can grow, causing the bi-film defects to sediment more rapidly. This process results in a cleaner melt, which can then be transported for casting through the launder at a specified flow rate, such as 180 kg/h in these initial trials. Higher rates of interest to industry are planned.

The particles used in the simulation were of various sizes: 25 µm, 50 µm, 100 µm, and 1000 µm. They were modelled with three different densities: 2000 kg/m³ to represent porous alumina or SiO_2 (and any low-density impurities) in the dross, 3990 kg/m³ to represent bulk alumina and 3450 kg/m³ to represent intermetallics. Except for Mg_2Si or SiO_2, the theoretical densities, Table 1, of most common inclusions in aluminium alloys are significantly higher than that of the liquid melt. These particles typically form during the latter stages of solidification, whereas $(Al,Si)_3Ti$ is expected to form before primary aluminium, as it nucleates on bifilms. Therefore, for comparison purposes, the simulation includes a lower-density inclusion (compared to the melt), which could represent floating dross before casting or ensure that the simulation remains realistic. However, the surface flux on the launder is expected to trap any floating bi-films that encounter it, drawing them into the flux layer due to capillary attraction forces. As a result, these bifilms will not be able to float to the exit of the launder. Over time, the accumulation of bifilms in the flux will require periodic renewal, as the increasing film content will raise the viscosity of the flux and inhibit any flow. Additionally, the drag from the upper and lower surfaces, as well as the walls, will further restrict movement within the thin flux layer, which is only a few millimeters thick.

Table 1: Theoretical densities of some inclusions in Al based alloys.

Inclusions	Density (kg/m^3)
$(Al,Si)_3Ti$	~ 3400
Mg_2Si	2000
Al_2Cu	4000
$FeAl_3$	3300
Al_3Ni	4100
Al_5Fe_2	4000
Al_5FeSi	3200
Al_8Fe2Si	3300
Al_6FeMn	3700
Al_2O_3	3950 to 4000

To assess the effectiveness of the process of sedimentation, “flux surfaces”[2] were used in the simulation. “Flux surfaces” are a special subset of baffles that have a fixed porosity equal to 1, meaning they are completely open to flow. These are special objects used to measure the flow of quantities through them. One “flux surface” tracked the number of particles generated and

[2] Not to confuse with the fluxing using salts.

entering the launder, while the other “flux surface” tracked the number of particles exiting the launder. This setup enabled the determination of the effectiveness of the sedimentation process by comparing the number of particles entering and exiting the launder.

Boundary- and Initial- Conditions

The boundary conditions for the simulation were provided by our industry partner, Sylatech. These conditions were based on physical measurements taken during melt holding within the launder system. The simulations then helped Sylatech to optimise some conditions or model setups for an effective melt cleaning process. This iterative approach ensured that the boundary conditions were realistic and that the simulations provided actionable insights for improving the melt delivery system. Sylatech's collaboration has been crucial in validating the simulation models and enhancing the performance of the melt cleaning process.

Results and Discussion

The simulations revealed that most of the particles having higher density than the melt effectively settle within the launder at the specified flow rate of 180 kg/h. However, those with lower density floated, and were carried away with the melt flow. These results indicate the need for further optimisation to enhance the efficiency of the sedimentation process. The simulations so far represent an initial exploration, requiring further simulation with more realistic initial and boundary conditions. The simulations were compared with - and without - the heat transfer activated, and the results varied significantly. The heat transfer plays a role in settling the particles.

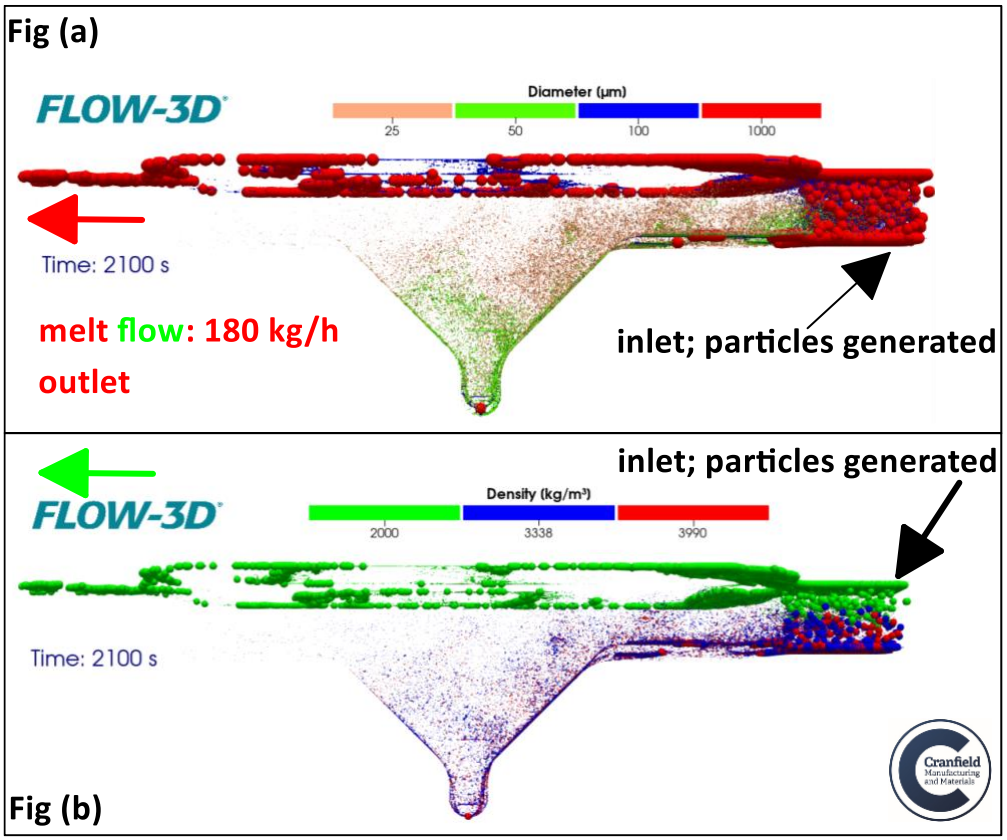


Figure 3: Simulation of melt flow with particles and heat transfer activated; a model simulation with particle sizes of 25 µm, 50 µm, 100 µm, and 1000 µm, with boundary and initial conditions as per Table 1. Colour codes for (Fig(a)) particles size and (Fig(b)) density. The melt flows from right to left, originating from the point where the particles are generated.

Figure 3 (Please note: A simulation video will be presented during the conference to illustrate the natural convection of these particles.) shows that at approximately 2000 s, particles reach the exit end of the launder unless they sediment beforehand, depending on particle size and density. Particles of 1000 µm and lowest density reach the exit-end. Most of the particles, that are higher density than the melt, sediment before reaching the exit-end, indicating they are mostly trapped within the basin section (the lowest section) of the launder. Most of the particles, being of higher density than the melt, tend to sediment before reaching the exit-end, indicating they are largely trapped within the basin section of the launder. The sedimented particles are expected to have a lower restitution coefficient, which causes them to lose energy and settle within the basin. However, to address potential re-entrainment of particles due to changes in flow rate, it is important to monitor and control these fluctuations to minimize disruption of the sedimented particles. Therefore, the initial selection of particle size is vital for the optimum performance of the intended purposes, which is to attract other impurities (Al_2O_3), grow, and settle. All lower density particles take about 2000 s to float and reach the end, travel through the launder, and reach the exit end. In contrast, particles with higher density than the melt density at the temperature remain suspended in the melt through the launder. These smaller particles are mostly trapped within the lowest section of the launder. Therefore, the selection of particle size is vital for the optimum performance of the intended purpose. Note: In the simulation, the temperature at the top of the launder is maintained at a constant 650 °C, which is achieved using heating elements in practical applications.

Mesh Size and Simulation Details

In computational fluid dynamics (CFD) simulations, the mesh size is a crucial parameter that significantly influences the accuracy and stability of the results. Errors in both measurements (e.g, a fluctuating temperature of the melt pool, using a K-type thermocouple, at elevated temperature may be up to ±5 %) and simulations or computations are inevitable; therefore, utilising a Pareto front in multi-objective optimisation is essential for achieving realistic simulation outcomes. For example, in Flow3D simulations, a coarse mesh size can lead to issues such as "excessive pressure error" or "convective flux exceeded stability limit" particularly when simulating the exit of this launder with dimensions around 100 mm × 100 mm. To mitigate these errors, a mesh size of 6 mm was deemed appropriate, determined through multiple iterations of simulations with various mesh sizes. Additionally, the frequency of output file generation can result in large file sizes, which pose challenges for post-processing. Consequently, both software-related parameters, and boundary- and initial-conditions were optimised to ensure a reasonable realistic outcome of the simulations. This careful balance between mesh size and computational parameters is critical for the successful implementation of CFD simulations in this complex system.

Challenges and Solutions

During the project (both practical and simulation conditions), several challenges were

encountered, including, variability in particle sedimentation due to flow rate changes. Difficulty in capturing smaller particles or lower density particles within the launder. Adding heat sources and conducting heat through the gas medium is computationally challenging. To tackle this, a constant temperature was set to the Z-max boundary (top surface). This approach simplified the simulations but may be refined in future simulations for more detailed input and outcomes.

The output data size is a function of data generation frequency, and it also consumes computation time. With the 32-core software license on the HPC, the output frequency was heavily increased to tackle this challenge. The output data/file size affects the post-processing time, as loading the file into Flow3D POST sometimes fails. To face this challenge, a better post-processing workstation may be suitable or securing simulation time (similar to funding application) with UK's national computation facility (ARCHER2); maybe possible for the later part of the project time line.

Increasing the number of cores on the Flow3D software license will help speed up the simulation, especially when altering boundary conditions, flow rates, and initial conditions for the same setup and conducting multiple simulations to identify the optimum parameters. For the initial period of simulation, it was manageable, but it will be a vital part for the next step of the simulation. Therefore, the next step in the simulation should follow according to the Table 2. Further simulations with varying flow rates and boundary conditions are planned, Table 2, to optimize the launder design and to address these challenges.

Table 2: Simulation Boundary and Flow Conditions (**current** and planned).

Parameter	Suggested Value	Rationale/Objective	Expected Outcome/Study Aspect
Flow Rate	100 kg/h, **160 kg/h**,[3]	To study the effect of varying flow rates on particle sedimentation	Determine optimal flow rate for maximum sedimentation efficiency
Particle Sizes	10 µm, **25 µm,** **50 µm,** **100 µm**, 500 µm, **1000 µm**	To assess the impact of different particle sizes on sedimentation	Identify size threshold for effective sedimentation
Particle Densities	**3990 kg/m³ (Alumina),** **3338 kg/m³ (Iron Intermetallics)** 2560 kg/m³ (solid	To confirm findings with different particle densities	Validate current density assumptions

[3] Our specific condition for this aerospace casting application involves a flow rate of 160 kg/h, which is significantly lower than the typical industrial DC-casting launder rates of 20000 kg/h to 50000 kg/h. This lower flow rate is tailored to meet the specific requirements of the aerospace alloy casting process. While the current paper focuses on these conditions, it is acknowledged that future simulations could explore a broader range of flow rates if needed.

	mixture of alumina and aluminium)		
Lower Density Particle	**2000 kg/m³**	To understand dross formation and accumulation	Compare sedimentation and floating behaviour of lower density particles
External Temperature	**180 °C**,[4] 220 °C	To examine the influence of external temperature variations	Understand how temperature affects melt cleanness
Initial Melt Temperature	630 °C, **650 °C**, 670 °C	To explore the effect of fluctuation in initial Al alloy's melt temperature	Optimise initial conditions for best melt quality
Atmospheric Pressure	1.2 atm, **1 atm,** 0.95 atm (measurement required)	To investigate the impact of slight pressure variations especially due to Ar flow or thermal effect	Assess the role of pressure in particle sedimentation
Additional Factors	Varying flow patterns, launder geometry changes (when occurs)	To refine the model with more realistic conditions	Enhance simulation accuracy and predict real-world performance
Argon Gas Application	Introducing Ar gas over the top surface	To minimise chemical reactions with atmospheric gases and isolate the melt from air, and to understand the heat absorption by Ar gas; it has lower specific heat compared to air but affect in a flowing condition.	Optimise flow rate to avoid excessive heat dissipation from the melt surface
Mass particle coefficient of restitution	0, 0> and <1 1> **1**	This means that the particles bounce back when colliding with wall; zero value means it will stick with the wall when they first become contact with the wall. The launder interior is coated with BN to prevent sticking,	Need to adjust this value for a realistic outcome; must be 0> and <1.

[4] This is the external temperature of the launder measured during melt holding using a thermocouple, and it is set as a condition in the simulation.

		otherwise the whole process would become unworkable within a few hours.	
Simulation Condition :cfpk	0.01 (software or CFD related parameter)		
Output file size			>50 GB
Number of output states:			- From 0 s to 10 s: every 1 s - From 10 s to 100 s: every 10 s - From 100 s to 1000 s: every 100 s - From 1000 s onwards: every 100 s Actual wall time on HPC: up to 7 days Simulation time: up to 3000 s

While the specific design of the launder system developed for melt cleaning and delivery is proprietary, this paper presents the simulation results and performance analysis derived from the system. The focus is on the outcomes of the simulations rather than the detailed design itself.

The results from the simulations highlight the key aspects of the sedimentation process within the launder system for aerospace-grade aluminium alloys. The simulations demonstrated that particles with a density higher than that of the melt (e.g., alumina and intermetallics) sediment effectively within the launder under the specified flow conditions. As the melt travels at a rate of 180 kg/h through the launder, larger particles (100 μm) and those with higher densities (e.g., 3990 kg/m³ for bulk alumina) tend to sediment before reaching the exit end of the launder.

In contrast, lower-density particles, such as porous alumina with a density of 2000 kg/m³, are unlikely to settle and are instead carried through the launder by the melt flow. This suggests that while the current launder design is effective for removing denser impurities (than the melt), there is a need for further optimisation to target lighter inclusions. In order to address the challenge of lighter particles, which naturally float to the surface due to their lower density compared to aluminium, adjusting parameters such as the apparent particle density, flow rate, initial particle size, and temperature may enhance sedimentation efficiency. These adjustments can help simulate conditions where lighter particles behave like heavier inclusions, aiding their removal from the melt.

Additionally, the activation of heat transfer, from melt to launder to air, within the simulation significantly impacted particle behaviour. The results showed that heat transfer plays a critical role in assisting sedimentation, particularly for larger (~ > 50 μm) and denser (than the melt) particles. Without heat transfer, sedimentation rates were considerably slower, indicating that precise thermal control within the launder system is essential for efficient melt cleaning.

Future simulations will explore varying boundary conditions, such as lower flow rates and additional particle sizes, to optimise the sedimentation process further. The next phase of trials will focus on refining the launder geometry and flow conditions to enhance the capture of lower-density particles, ultimately aiming for a cleaner melt that aligns with aerospace industry standards for alloy purity and performance.

Conclusions

The results are expected to provide a comprehensive understanding of the melt cleaning process for sustainable aerospace structural castings and design of a new launder system that could help the foundry industry to provide a greener solution for the aerospace industry to align with the net-zero target.

This study demonstrated the effectiveness of using a launder system for the sedimentation and removal of impurities from aerospace-grade aluminium alloy melts. The simulations, conducted using Flow3D software, revealed that particles with higher densities, such as alumina and intermetallics, settle efficiently within the launder under the specified flow and thermal conditions.

The results underline the importance of precise control of flow rates, particle sizes, and thermal management to achieve optimal melt cleanness. Heat transfer was shown to significantly influence particle sedimentation, highlighting its critical role in melt processing. This is what causes the convective flow within the launder system and accelerate the sedimentation of these inclusions.

While the current launder design is successful in removing larger, heavier particles, future work will focus on refining the design and processing conditions to enhance the sedimentation of lighter inclusions or preventing the formation of these inclusions. This optimisation will contribute to the development of cleaner aluminium alloy melts, supporting the aerospace industry's goals of improved material properties and more sustainable manufacturing practices.

- The launder system effectively removes higher-density particles (e.g., alumina and intermetallics) from aerospace-grade aluminium alloy melts.
- Simulations using Flow3D showed that denser, than the melt, particles settle efficiently under the specified flow rate (180 kg/h) and thermal conditions.
- Lighter particles, such as porous alumina, present challenges in sedimentation and require further optimization of the system's flow rate and temperature and environmental controls to reduce the formation.
- Heat transfer, in causing convective flow within the launder, has a crucial role in enhancing particle sedimentation, emphasising the need for precise thermal management.
- The current launder design, together with the initial- and boundary- conditions performs well for larger (~ >50 μm) and heavier particles but will need refinement to improve the removal of lighter impurities.
- Future work will focus on optimising the launder geometry, flow conditions, and processing parameters to achieve cleaner melt for finer particles.

- These improvements will support the aerospace industry's goals for higher material quality and sustainability in aluminium casting processes.

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