

Modeling and Simulation of Cold Hearth Continuous Casting of Titanium Alloys

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Abstract

In the present study, an alternative sustainable method of manufacturing of Ti6Al4V alloys from industrial scraps/swarfs is discussed. CFD modeling and simulation of cold hearth continuous casting process is done using FLOW-3D TruVOF and FAVOR techniques. A High-Performance Computing is utilised to optimise the computing resources to simulate the hydrodynamic and thermal behaviour of the liquid metal. Simulations with different superheating temperature is conducted to understand the flow properties and solidification. These findings provide valuable insights into understanding of flow properties and thermal distribution for reliable molten metal delivery contributing to efficient recycling and sustainable manufacturing processes.

Keywords: Aerospace, Titanium alloys, continuous casting, CFD modeling, simulation, sustainability, supercomputing

1. Introduction

Titanium alloys find predominant usage in Aerospace and Biomedical applications. It is evident that the demand for Ti-alloys per commercial aircraft has risen from approximately 9% in 1995 to around 14% in 2015, marking a 50% increase since 1995. A significant surge in the supply of Ti-alloys to the Aerospace industries has been observed. This surge has consequently led to an upswing in the mining of Titanium ores for Titanium sponge production, catering to the raw material manufacturing of Titanium, followed by subsequent production of various Ti-alloys. Demand is on the rise adding significant cost implications to the production[1]. Aerospace parts require stringent inclusion controls because of the premature failure of rotating parts due to presence of HDI/LDI inclusions[2]. Titanium remelting is widely used to get rid of the inclusions such as High-Density Inclusions (HDI) such as WC and/or TiO₂, and Low-Density Inclusions (LDI) such as titanium enriched with interstitial elements such as N₂ and/or O₂[3]. Hearth Melting (HM) techniques using either vacuum or inert gas atmosphere are widely adopted in industry due to their potential for elimination of HDI, and dissolution of LDI resulting from the longer residence time of liquid metal in a water-cooled copper crucible [3–5]. The conversion of raw Ti alloys into machined parts constitutes only 50% of the parts' weight, with the remaining 50% discarded as swarf (cutting chips and turnings). Consequently, this leads to a low buy-to-fly ratio for the machined parts. In certain instances, within the aerospace industry, scrap can make up as much as 90% of the machined parts. A noteworthy example is the generation of 100 tons of Ti alloy scrap from a 120-ton Ti alloy ingot used in the manufacturing of Boeing 787 airframes [6]. Similarly, for biomedical applications such as machining knee parts, a substantial 80% of the machined parts' weight is scrapped [7]. There is a strong demand to improve the circular economy and sustainability of the aerospace parts. Recently, attention is given to improve recycling of the titanium scraps/swarfs using different techniques. Techniques like (i) solid to solid state transformation such as Conform[8] and FAST forge[9], and (ii) continuous casting using high energy sources such as laser beam melting [10], electron beam melting [11,12], and plasma arc melting [3,13] are adopted to different titanium alloys. The selection of these techniques depends on the type of titanium alloys and the volatile nature of the chemical composition, intricacy of the components and the scale of production.

The quality of manufacturing scraps depends on the type of milling operation used for machining. Presence of contamination not only affects the quality of the melt but deteriorates the mechanical properties substantially. Unlike water cooled copper crucible for hearth melting and refining, recent work suggests the use of titanium as a crucible material for refining Ti sponges and other forms[13]. Also, the risk of copper contamination during melting or fluid residence time is eliminated. The possible impurities arise from conventional machining are due to the interaction between cutting fluids and cutting tools. However, recent

cryogenic machining developments reduces the likelihood formation of such impurities on the machined scraps/swarfs [14]. Experiments on a bulk scale model considers different heat transfer phenomena such as conduction, convection and radiation. The high reactive nature of the liquid titanium makes it hard to use any refractory material for melting. Hence, water-cooled copper crucible is usually made for hearth walls. Although there is no accurate data available for heat transfer coefficient of water-cooled copper crucible, Fourier heat conduction models used to compute thermophysical properties [15]. Also, modeling of the plasma torch is quite complicated due to the interaction between electromagnetic stirring, blowing of the torch and the hydrodynamics of the liquid metal are not yet been explicitly studied [16]. To improve the numerical simulations, improvements such as volume of fluid technique to account two fluid phases, impingement of plasma jet and the movement of torch and computing close to real heat transfer coefficient are suggested. Since most of these studies are on atleast pilot scale experiments but no micro scale experiments have been reported so far.

In this work, the development of CFD models considering the micro scale experiment set up for the recycling of titanium scraps by remelting the titanium scraps in a compacted solid briquette form for continuous micro-casting is discussed. Schematic diagram of remelting of Titanium solid is shown in Figure 1 (a) which is adopted from titanium refining technologies[3,13]. This model contains two stages (stage 1 and stage 2) and the mass momentum at required liquid/solid temperature (T_{momentum}) is given in stage 1 and the liquid metal will flow through stage 2 to spout and for further processing. Given the high purity of swarf with no or negligible contamination, an alternative material for the crucible is chosen such as Ti64 given the same Ti64 scrap is to be melted for continuous delivery of liquid metal [13]. Low thermal conductivity and higher specific heat capacity of Ti64 prevents the loss of thermal energy contained in the crucible which is beneficial to reduce the heat input to melt the swarfs. However, the crucible temperature needs to be monitored continuously to minimise the melting. This can be achieved by (i) optimizing the heat input/energy, and (ii) providing suitable insulating materials. Typically, 50 °C superheating is employed above the liquidus temperature to maintain the liquidity of Ti64 alloys [17]. The minimum energy required to maintain the liquid for continuous delivery of the molten metal to the destination is computed by the simulation. Thus, the simulation results will be used to further iterate the model to optimize the energy requirements, fluid flow, heat transfer and to minimizing the defects. The simulated results will be validated using the experimented results and a correlation will be obtained to optimize the energy requirements which is our future study. The assumptions considered for the simulation are the (i) homogeneous heat transfer between heat source and the surface the solid/liquid phase and (ii) predominantly conduction heat transfer because of the micro-scale model. However, appropriate boundary conditions are applied assuming the process takes place in an inert atmosphere and the simulation results are obtained using a pioneer CFD software, FLOW-3D with the user defined functions [18].

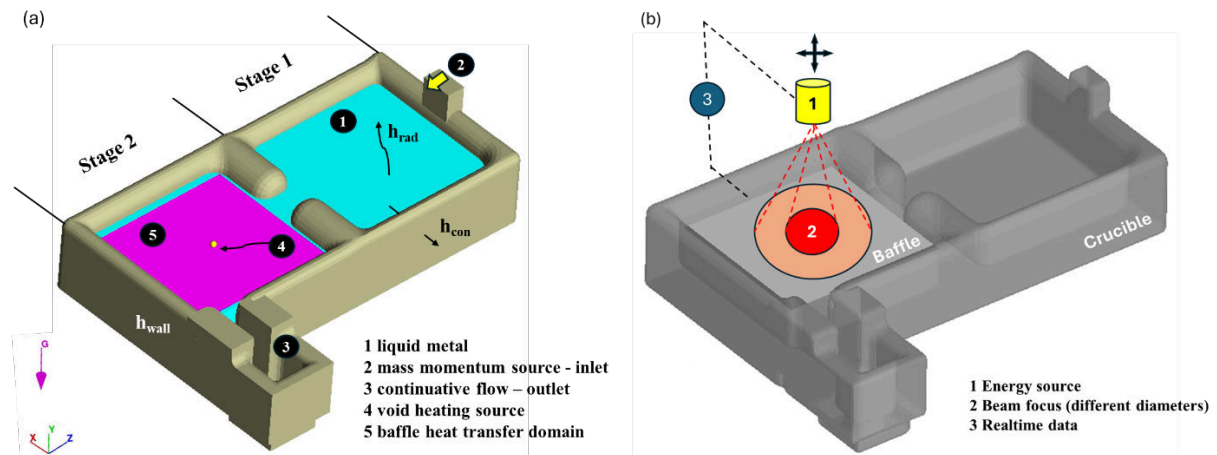


Figure 1 (a)3D model of the 2-stage crucible indicating initial and boundary conditions.
(b)FAVOURised model and heating source configuration

2. Mathematical Modeling

In the present study, FLOW-3D's volume of Fluid (VOF) technique is employed to solve the numerical simulation of the fluid dynamics and heat transfer under transient conditions. The mathematical equations used in the TruVOF method to solve fluid dynamics problems involve a combination of partial differential equations (PDEs) and algebraic equations. The TruVOF method specifically involves advanced techniques for discretizing the volume fraction equation and accurately capturing the interface dynamics. Also, FAVOR (Fractional

Area/Volume Obstacle Representation) technique is used to model complex geometries by calculating the fractional volume of cells occupied by solid obstacles, enabling accurate flow simulations without requiring a body-fitted mesh. This approach enhances computational efficiency and maintains accuracy in fluid-structure interactions[18].

The mathematical model for the plasma arc melting for an incompressible fluid is described by three major components such as mass, momentum and energy conservation. The continuity equation for the mass conservation in the crucible/hearth is given as

$$\nabla \cdot u = 0 \quad \text{Equation 1}$$

where u is the velocity vector of the fluid.

The momentum conservation component is

$$\rho \left(\frac{\partial u}{\partial t} + (u \cdot \nabla)u \right) = -\nabla p + \mu \nabla^2 u + F_g + F_s \quad \text{Equation 2}$$

where ρ is the density, t is the time, p is the pressure, μ the dynamic viscosity, F_g is the gravitational force which includes body force and buoyancy, F_s is the surface force which includes surface tension, thermal Marangoni shear stress.

The energy conservation component is,

$$\rho \left(\frac{\partial h}{\partial t} + (u \cdot \nabla)h \right) = \nabla \cdot (k \nabla T) + S \quad \text{Equation 3}$$

where h is the enthalpy, k is the thermal conductivity, T is the temperature and S is the heat source term which includes heat loss. Also, the liquid fraction (β) in the molten pool is given as

$$\beta = \frac{T - T_{sol}}{T_{liq} - T_{sol}} \text{ if } T_{sol} < T < T_{liq} \quad \text{Equation 4}$$

where T_{sol} is the solidus temperature, T_{liq} is the liquidus temperature.

$$\beta = 0 \text{ if } T < T_{liq}$$

$$\beta = 1 \text{ if } T > T_{liq}$$

Boundary conditions:

(i) At bath surface:

Thermal emissivity (ϵ) of the liquid Ti64 varies as a function of temperature and in the present simulation the influence of widely reported emissivity ($\epsilon = 0.2$) value is considered. The heat source was attached to the baffle and the defined heat source distribution (varying temperature and time) is applied to maintain the required temperature. The high heat transfer coefficient (HTC) ranging between 10^5 - 10^6 W/m²/C was assigned to make sure the melting occurs rapidly in the crucible. The heat flux distribution from heat source to the liquid metal surface was uniform across the liquid Ti or solid Ti (raw materials such as swarfs or blocks) domain.

$$q_{surface} = q_{heat source} - q_{con} - q_{rad} \quad \text{Equation 5}$$

where $q_{surface}$ is the heat flux at the bath surface from heat source, and $q_{heat source}$ is the heat flux from the heat source, respectively. The radiation heat transfer (q_{rad}) from a surface with area A for a given surface temperature can be found using q_{rad} . However, this radiation model does not include view factors.

$$q_{rad} = \sigma \cdot \epsilon \cdot (T_{surf}^2 - T_{wall}^2) \quad \text{Equation 6}$$

where, σ is the Stefan-Boltzmann constant ($5.6697 \cdot 10^{-8} \frac{W}{m^2 K^4}$), ϵ is the emissivity of liquid titanium, T_{surf} is the surface temperature of the metal, T_{wall} is the wall temperature.

(i) At walls:

Fourier heat conduction was applied to compute the heat transfer coefficient between the crucible wall and the liquid metal. No-slip boundary condition was applied. The heat transfer coefficient of the liquid metal and the wall is computed for range of temperature such as 1660 °C, 1670 °C and 1700 °C using the following equation.

$$q_{con} = h_{con} \cdot A \cdot (T_{liq} - T_{sol}) \quad \text{Equation 7}$$

3. Numerical simulation

A Rectangular mesh with the uniform mesh size of 60 μm is used to uniformly mesh the entire domain to capture the localised thermal history and fluid dynamics of the melt. The simulations have been run on a 32-core license solver in Delta-2 High Performance Computing (HPC) facility at Cranfield university, UK. This will further breakdown the complex problems into multiple parallel processing thus improving the computing efficiency. But, still on an average each computation time on a HPC takes ~ 48 h to simulate an actual simulation time of 100 seconds. The computational output file is chosen for every 1 second and a FLOW-3D post was used for postprocessing.

Thermophysical parameters used for Ti6Al4V (Ti64) is given in Table 1 and the initial and boundary conditions of the simulation are given in Table 2. Although, the calculated flow properties such as Reynolds number (~ 616) and Nusselt number (~ 6.3) is for laminar flow, a turbulent model using RANS (Reynolds-Averaged Navier-Stokes) k-e is considered to predict the localised turbulent properties. Given this a higher computation time is inevitable.

Table 1 Thermophysical process parameters

Parameters	Values	Unit
*Density,	4420	kg/m^3
*Viscosity, μ	3.25×10^{-3}	kg/m/s
*Specific heat, C_p	546	$\text{J/kg/}^\circ\text{C}$
*Thermal conductivity, k		
k @ 25 $^\circ\text{C}$	7	$\text{W/m/}^\circ\text{C}$
k @ 1700 $^\circ\text{C}$	34.6	$\text{W/m/}^\circ\text{C}$
Liquidus temperature, T-liq.	1650	$^\circ\text{C}$
Solidus temperature, T-sol.	1600	$^\circ\text{C}$
Latent heat of fusion, L_f	286	kJ/kg
Thermal expansion coefficient	9.0×10^{-6}	K^{-1}

*Temperature dependent values are used in the simulation

Table 2 Initial and boundary conditions

Parameters	Values	Unit
Pressure	101325	Pa
Void (Argon) temperature	25	$^\circ\text{C}$
Cell size	60	μm
Total Cells	~ 0.8 million	nos.
Simulation conditions		
Case 1: Melting (Stage 1 and Stage 2) without mass momentum source	25	$^\circ\text{C}$
Case 2: Melting (Stage 2) and Continuous casting with inlet mass momentum temperature		
T_{momentum}	1660, 1675, 1700	$^\circ\text{C}$
m_{momentum}	13	g/s

In general, the release of latent heat is given as a function of linear temperature for some materials. However, for the present case, it can be defined as a tabular function of temperature. This can be done in the form of either specific energy vs. temperature or solid fraction vs. temperature. The melting of the solid phase is achieved by baffle type heat transfer with a high HTC. The position of the baffle is shown in Figure 1 (a) and (b). The baffles can be customised to the intended locations based on the thermal history. Also, the void is set with the required heat transfer coefficient to minimize the melting duration. Since baffles are treated as having no thickness and consequently no heat capacity, the heat transfer rate depends only on the instantaneous fluid temperatures on either side of the baffle. The energy required to melt, and superheat is computed using first order thermodynamic principles and the numerical results are compared to optimize the energy inputs and minimize the losses. Assumption considered is no radiation losses and loss of alloying elements. However, evaporation losses can be included by modeling relevant thermophysical properties.

4. Results and Discussions

Case 1: Modeling of melting

The melting simulation results are shown in Figure 2. The maximum liquid bath surface temperature of 2178 °C and 1795 °C is achieved for the heat source temperature of 2500 °C and 2000 °C, respectively. The maximum wall temperature of 1560 °C is obtained at higher heat source temperature of 2500 °C. The variation in thermal energies, fluid and wall temperature is caused by the heat distribution/duty cycle of the heat source temperature/time. A proper insulation or cooling mechanism is necessary to maintain the crucible/wall temperature. In the present case, baffle is placed in both stage 1 and stage 2 (Figure 1) of the crucible to compute the energy required to melting and the power is derived thereafter. This energy represents only the surface melting from the baffle position. This is considered to melt any low-density inclusions floating atop and prevents the heating of the crucible wall. The energy required to melting the mass of 120 g according to first order thermodynamics principles is ~ 207 kJ which agrees with the simulated thermal energy of ~ 206 kJ at time is zero when the initial liquid is set to liquidus temperature at the start of the simulation. As the simulation proceeds, the heat losses such as conduction happens predominantly in the present case due the static condition of the melt. Thus, resulting in higher energy required to melt the complete mass. This can be achieved by setting the heat source to higher temperature and a higher HTC or by changing the baffle configuration from sheet into cylindrical.

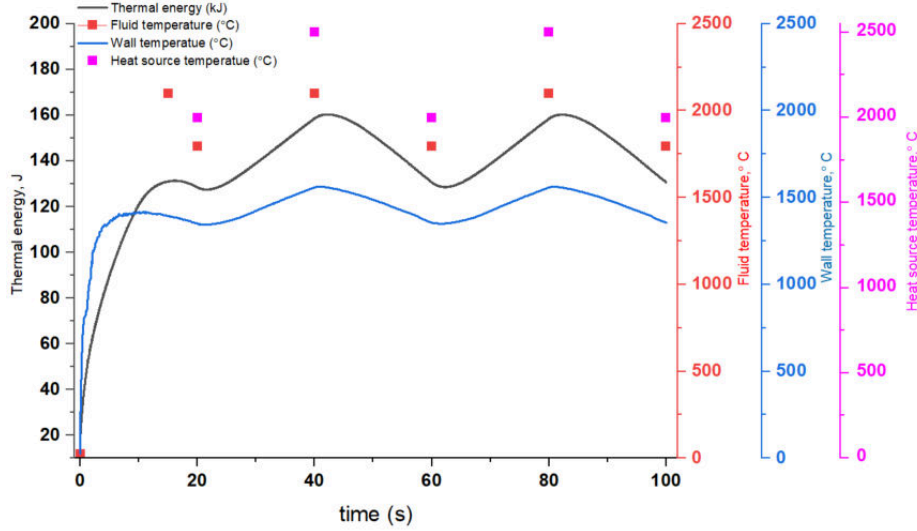


Figure 2 Simulation results using static melting conditions without mass momentum source

The partially melted profile of the solid Ti block is shown in Figure 3 (a) in which the surface temperature of the liquid bath indicates 1795 °C at 100 s. The corresponding solid and liquid fraction is 0.682 and 0.318, respectively as shown in Figure 3 (b). The power is computed by taking the slope of thermal energy which is $\sim 8.5 \pm 0.2$ kJ/s at 15 s to raise the maximum bath surface temperature (2178 °C) as shown in Figure 3 (c). The variation in power requirements caused by the differences in fluid temperature which indicates less power is required when the bath surface temperature is higher and vice versa. In addition, the additional power required to raise the temperature from 1795 °C to 2178 °C is varying between 1.4-1.5 kJ/s.

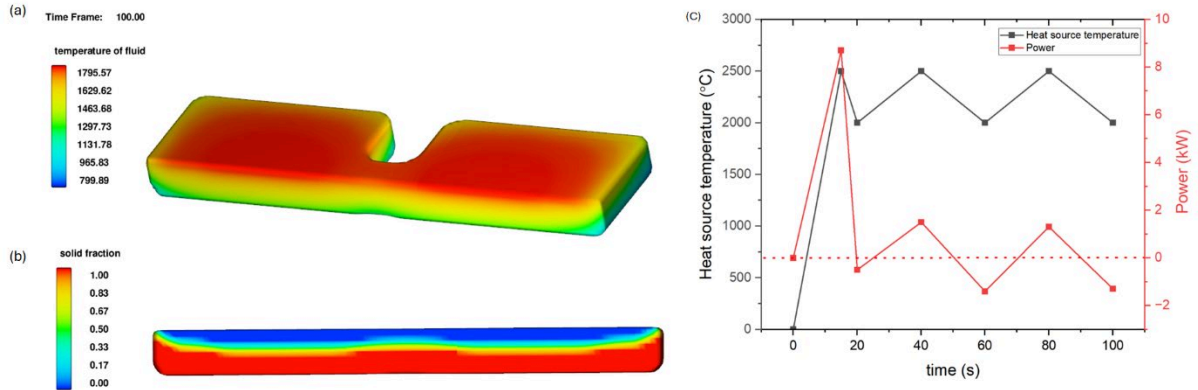


Figure 3 Sectional view along X-Z indicates (a) temperature profile of the fluid, and (b) solid fraction

Case 2: Modeling of Melting and Continuous Casting

In this case, the crucible is filled with the liquid metal at required T_{momentum} , and the mass momentum source is activated with the corresponding T_{momentum} . In addition, the heat source is applied only to stage 2 of the crucible. The purpose of this simulation is to optimize the heating source in stage 2 while stage 1 is assumed to be continuously supplied with corresponding T_{momentum} source and the energy lost from stage 1 to stage 2 is compensated by the stage 2 heating source. This thermal convection facilitates the sedimentation of HDI inclusions in stage 1 leaving LDI into stage 2 which will eventually get melted and the clean metal will be delivered through stage 2 spout to the intended application. An option of adding different multi-energy source can be considered depending on thermal history and the real-time data will be fed to the heating source to optimize the required power.

Figure 4 shows the liquid bath surface temperature and the flow pattern of the molten metal at different T_{momentum} . It can be easily seen from that for lower T_{momentum} the temperature gradient across the Z-Z is lower this will lead to a thicker mushy zone forming a hard skull layer at the bottom of the crucible. Further experimental validation is necessary to confirm the presence of HDI and other undesirable microstructural features. The maximum bath surface temperature of $\sim 1830^\circ\text{C}$ is obtained for T_{momentum} of 1700°C while the minimum bath surface temperature of $\sim 1816^\circ\text{C}$ is obtained for T_{momentum} of 1660°C . For a T_{momentum} of 1675°C , the surface bath temperature of $\sim 1821^\circ\text{C}$ is obtained. The entry and exit of the metal flow is highlighted by the white arrows (dashed) and the corresponding sectional views along Z-Z to represent the liquid/solid fraction is shown in Figure 5.

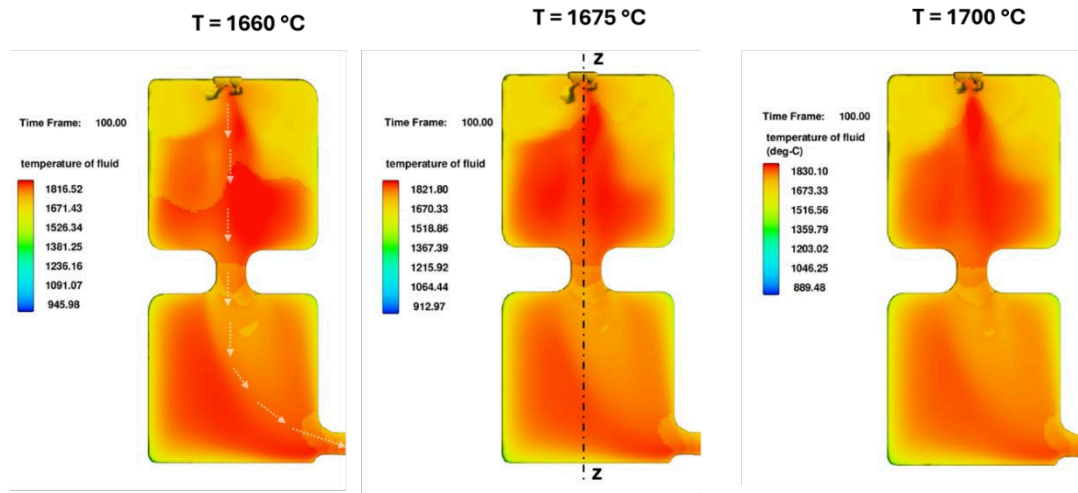


Figure 4 Surface temperature of the liquid bath with different mass momentum temperatures (1660, 1675 and 1700°C). Dotted white arrow indicates the flow of metal from the mass momentum source to the delivery spout. A high temperature gradient is noticed in stage 1 at $T = 1660^\circ\text{C}$ compared to the others

Figure 5 shows the variation in liquid and solid fraction as a function of different T_{momentum} temperatures. The liquid fraction of 0.156, 0.158 and 0.159 is achieved for T_{momentum} of 1660°C , 1675°C and 1700°C , respectively. The corresponding liquid to solid fraction ratio is 0.308, 0.302 and 0.29 for the increasing order of T_{momentum} . The skull length at the bottom of the crucible is measured to be higher for lower T_{momentum} of 1660°C (L1) compared with higher T_{momentum} of 1770°C (L2). The entry of liquid metal is observed with the initial solidification due to the immediate contact with the wall (dotted rectangle in Figure 5) and the corresponding temperature contour is shown in Figure 4. Such accumulation will likely increase the skull depth thereby reducing the liquid fraction. In such case, thermal gradients from stage 2 to stage 1 occurs via convection thereby liquid temperature is increased and the skull formation is reduced at higher T_{momentum} . The constant heat input in stage 2 prevents the solidification in stage 1. Otherwise, premature solidification starts from the stage 2 and the molten liquid metal will be piled up when the temperature reaches critical limit. In addition, this can be customised depending on the required melt quality. Any defects such as cold and hot spots, premature solidification due to temperature variation is detrimental to the continuous delivery of liquid metal at required temperature. Also, the minimum fluid residence is essential to get rid of any LDI inclusions which can be tracked using fluid tracer feature. Continuous melting and casting indicate that there is no turbulence flow and the local velocity of the molten liquid is $< 0.7\text{ m/s}$ (maximum), and the maximum wall shear stress during the simulation is 8 MPa. Furthermore, the temperature measurements at the delivery spout indicates that at higher T_{momentum} resulting in higher exit temperature of the melt making it as suitable for subsequent processing. Therefore, the optimization of T_{momentum} and heat source distribution will lead to a reliable molten metal delivery without turbulent characteristics.

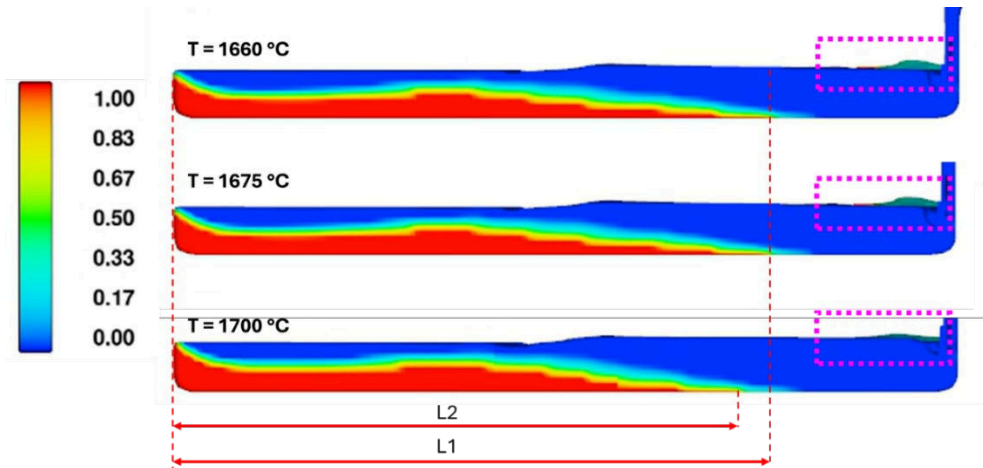


Figure 5 Sectional view along Z-Z of Figure 4 of different mass momentum temperatures (1660, 1675 and 1700 °C). L1 and L2 corresponds to the length of the solidified fraction at the bottom of the crucible. Dotted (rectangle) box indicates the accumulation of metal with varied liquid/solid fraction.

Conclusions

A potential micro melting and continuous casting of Ti6Al4V alloy has been successfully modelled and simulated using Flow-3D with the customization tools. The different heating models were configured to reasonably select the most accurate and reliable heat input to melting. However, further optimization on the heating source is needed to capture different heat source models such as laser, plasma or electron beam. Though present model considers thermal Marangoni stress the more accurate would be to include the shear stress acting on the surface of the liquid bath. This will be our next scope of work to incorporate them. Also, a similar approach to numerically model the heating source and the mass momentum source with the solid Ti64 blocks will be considered which is quite challenging.

Simulation of melting and using different mass momentum sources have indicated that both heat input (duty cycle) and a mass momentum source can be optimized to control the inclusions and enhance the metal delivery. This reduces the constant supply of power to melting thus reducing the energy consumption. In addition, optimum surface temperature of the bath and reduced skull length and depth can be achieved by conducting further simulations using different heat source temperatures and a reasonable heat transfer coefficient of both liquid, skull and the wall.

Furthermore, simulations such as complete melting in stage 1 and partial melting in stage 2 using different heat inputs are under study. Further studies on optimizing the mushy zone, minimizing the superheat required will be explicitly studied using iterative simulations and the experimental validation will be conducted to obtain the correlation and refine the simulation variables afterwards. The actual temperature measurements of the crucible and the power consumed will be studied. This will be helpful to optimize the duty cycle of the heating source to reduce the energy consumption and to minimize the required superheating. Life cycle assessment of the proposed method will be conducted to measure the sustainability index. Also, optimizing the CFD model, number of license solvers, and refining the simulation variables to increase the actual simulation duration will be perceived.

Funding

The project was funded by an EPSRC Programme Grant SAM (EP/W01906X/1). The authors would like to acknowledge the support from Cranfield University (HPC resources) and Flow Science, US.

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2025-03-03

Springer

https://doi.org/10.1007/978-3-031-80676-6_139

Mozhi Varman JPA, Sivarupan T, Georgarakis K, et al., (2025) Modeling and simulation of cold hearth continuous casting of titanium alloys. In: Light Metals 2025. TMS 2025 154th Annual Meeting & Exhibition, Las Vegas, NV, USA. The Minerals, Metals & Materials Series. pp. 1117-1124