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PHASE FIELD & MONTE CARLO POTTS SIMULATION OF GRAIN GROWTH AND MORPHOLOGY OF VERTICALLY UPWARDS CAST OXYGEN FREE COPPER

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Abstract: A 2-D Phase-Field coupled Monte Carlo-Potts model, using PhasePot of vertically upwards continuous casting (VUCC) of oxygen free copper (OFCu) was investigated to reveal the grain growth morphology and the withdrawal parameters required to produce a high-quality homogeneity within the grain structure. A dynamic moving reference frame was used as an approximation to the complex withdrawal parameters. The simulation results were validated alongside cast rod grain structures produced under the same cast parameters, at Rautomead Ltd on a RS080 VUCC machine.

KEYWORDS: CONTINUOUS CASTING – COPPER ALLOY – PHASE FIELD – MONTE CARLO POTTS – CALPHAD-GRAIN STRUCTURE – RAUTOMEAD LTD

INTRODUCTION:

Of high interest to Automotive and Power industries is the casting of pure oxygen free (0.001%) copper (OFCu) for use in electrical motors and wiring lines, respectively [1]. The highest quality casting with OFCu is achievable when vertically upwards continuous cast (VUCC) [2]. Withdrawal movements of the cast rod play a major role in as cast rod quality and ability to be downstream processed. To develop improved manufacturing processes and techniques, an accurate prediction of the cast behaviour is required. Traditional methods involve running a costly casting trial and evaluating retrospectively the outcome, however, coupled numerical simulations offer a lower cost alternative to predict the casting outcome, reducing the need for costly trials [3],[4].

The development of combined Phase-field and Monte Carlo-Potts models using PhasePot™ software provides an insight into the transient grain growth behaviour [5]. Phase-field simulation assumes the thermodynamic properties are dependent on the gradient of field variables and minimisation of these variables enables the movement of diffuse interfaces to be studied in simulations. The Potts model in combination with the Monte Carlo algorithm, as Monte Carlo-Potts, has been extensively used to model changes in polycrystalline materials. Combining the Monte Carlo-Potts method with the phase-field approach allows for efficient simulation of interface kinetics and diffusion of polycrystalline materials and has been applied in this study of OFCu casting. [6]

The current manufacturing capabilities for 8 mm diameter VUCC OFCu are 100 kg/hr or 4 m/min [7], however significantly higher outputs have been achieved and maintained within Rautomead Ltd at the expense of cast rod quality. Continuous forward withdrawal of cast bar has never been achieved empirically at 4m/min. This means the cast bar is subject to discrete time-based movements referred to as a withdrawal pattern or parameters. These parameters have a significant effect on the internal structure of the as cast product, and in turn the downstream process ability of the product. This study investigates the influence of withdrawal parameters on the homogeneity of the cast grain structure, along with their distribution within the casting die for two different simulation parameters, the results of which are contrasted against known casting behaviours.

EXPERIMENTAL

The commercially available Phase-Field (PF) coupled Monte Carlo-Potts (MCP) software PhasePot was used to simulate the VUCC of OFCu. The effect of thermal distribution throughout the withdrawal pattern has been investigated and a moving frame rate approximation has been used to approximate the complex movement of the rod. These two assumptions permit the simulation to be efficient while maintaining efficacy. This allows qualitative and quantitative analyses of the grain morphology and withdrawal parameter relationship. The boundary conditions for the PF/MCP simulation have been based on the results from reference [8,9], which describes the fluid and thermal profiles of the Rautomead Ltd casting setup including the dynamic withdrawal movements. Fig. 1 illustrates the casting setup for both the physical and the CFD model from reference [8,9], overlaid by the hatched rectangle is the region of interest for this study.

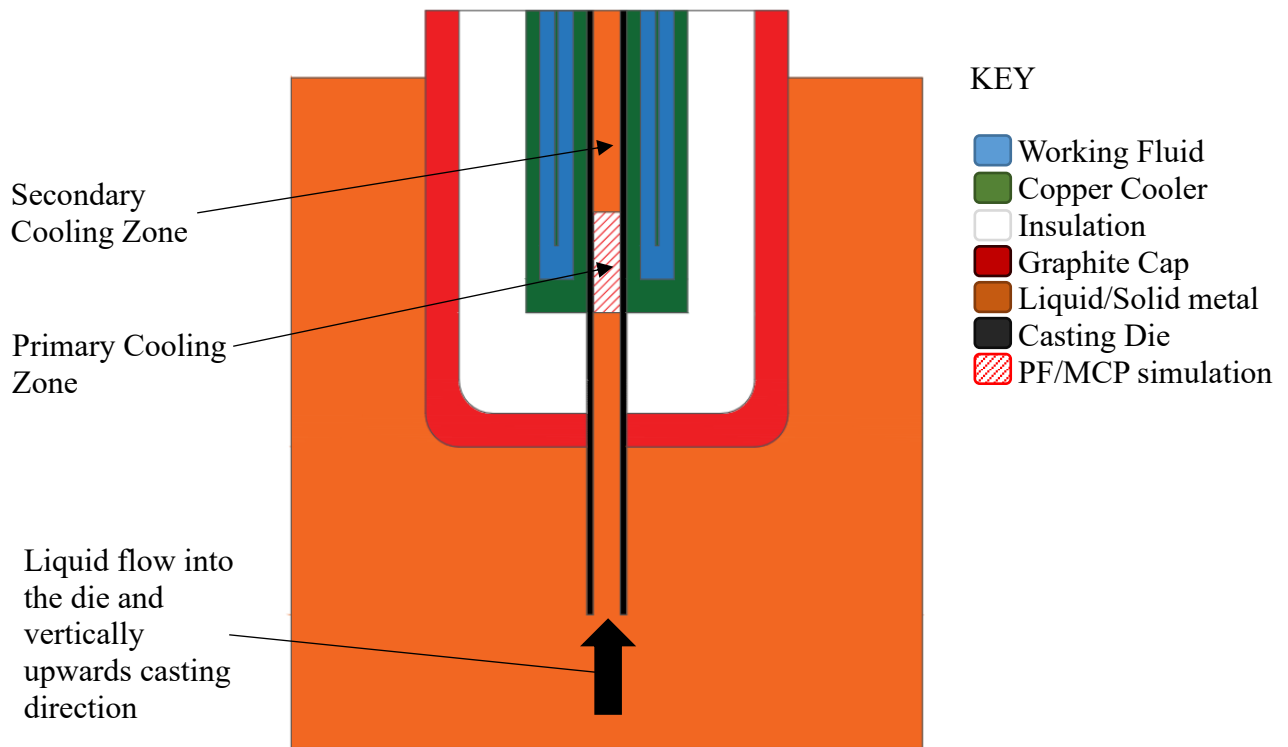


Figure 1 – Schematic diagram of VUCC with location of Phase-Field coupled Monte Carlo-Potts simulation

Unlike in the steel industry [10], the majority of solidification within copper and copper alloys occurs in the primary cooling zone, located within the die around the onset of the water cooling, highlighted as hatched rectangle in Fig.1. For this reason this small region was selected as the focus of this study. [2]

The simulations were performed on a 650x160 grid, with a grid cell size of 0.05 mm, and a time increment of 1500 ns. By iteratively manipulating the speed of the moving frame rate in conjunction with the number of time increments, the dynamic withdrawal of the rod can be resolved.

The simulation model was set up with a single Phase-field parameter where the temporal evolution of the phase-field variable was calculated with an Allen-Cahn formulation. Orientation was calculated with a cellular automata algorithm and heat transfer calculated using the heat equation[12]. Although nucleation sites can be randomly distributed these were not included. At this time, the PhasePot software cannot resolve both melting and nucleation sites simultaneously, therefore melting (or re-melting) was considered more significant based on previous work in reference [8,9].

This investigation focusses on the discretised motion of the withdrawal parameters and the resulting castability and quality of the rod. Cast rod was produced at Rautomead Ltd in Dundee on a RS080 VUCC machine to compare and validate the simulated results. Details of the successfully cast parameters are displayed in Table 1. The samples were prepared for analysis under a (Spectrographic, NMM-800RF) optical microscope by grinding, polishing and etching according to [11]. Parameters A-E (Table 1) are all forward-stop motion profiles (see fig. 2 for details) containing a forward move distance and a dwell (stop) time. Details of these parameters can be found under the 'Discretisation' heading in Table 1. Parameter F had no dwell, with forward motion only. These same parameters were applied as boundary conditions within this simulation study.

Table 1. – Casting parameters

Parameter Identification	Average Velocity (m/min)	Output Rate (kg/hr)	Discretisation (pull distance, dwell) time)
A	4.0	108	4.6mm, 0.034s
B	4.0	109	8.5mm, 0.059s
C	3.5	96	8.5mm, 0.076s
D	3.0	81	18.5mm, 0.301s
E	3.6	97	4.7mm, 0.021s
F	5.0	134	Upwards motion vertically only

SIMULATION RESULTS

Average Temperature and Solid Fraction

As the motion of the rod is dynamic, the average temperature will cyclically fluctuate for each of these simulations. Therefore, the average temperature between movement and dwell over the entire computational grid has been monitored, until the individual simulation reached an equilibrium condition. Equilibrium conditions were defined as the average temperature (over the computational grid) achieving a regular oscillation with the movement pulses. The equilibrated average temperature increased with casting rate, whereas the average solid fraction decreases with casting rate see figure 2. This can be attributed to the inflow of superheated liquid (> 1084°C Cu liquidus) metal during the movement which is subsequently solidified during the dwell period. As the casting rate is increased less time is available during the dwell to remove the energy before the next pull, Hence the increase in average temperature with casting rate, see figure 4 below.

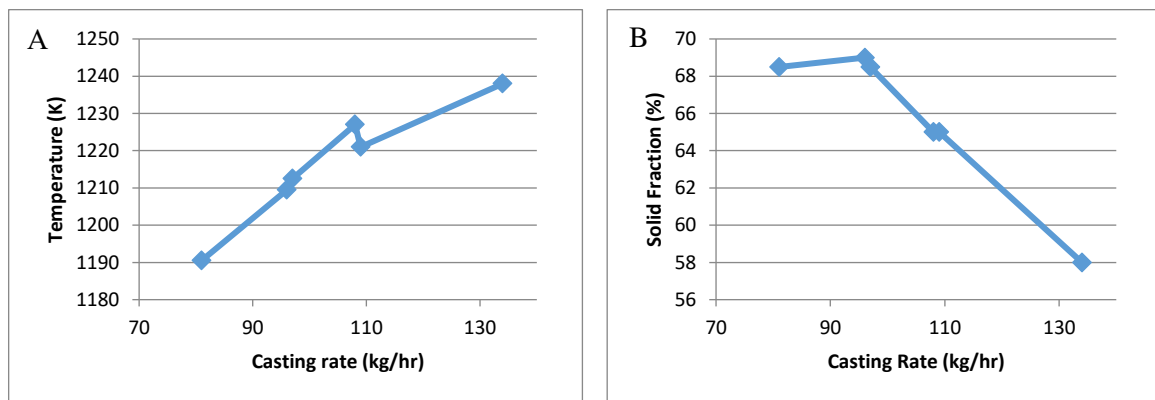


Figure 2 – Plots of simulated a) average temperature measured over primary cooling zone and b) average solid fraction

(%), measured over primary cooling zone; for all casting speeds.

Discretization

Displayed in Fig 3. are the simulated grain grow structures and their subsequent transient behaviours, occurring within the primary cooling zone (see Fig 1), for parameters A and D (see table 1). These parameters were chosen as they displayed the most distinct difference in dynamic grain morphology out of the parameters tested within this work. The graphs have been formed by plotting the phase-orientation of each cell over the computational grid between 0.9 and 1. This shows both the solid-liquid interface (liquid: black, solid: white), and the individual boundaries between differing grain orientations.

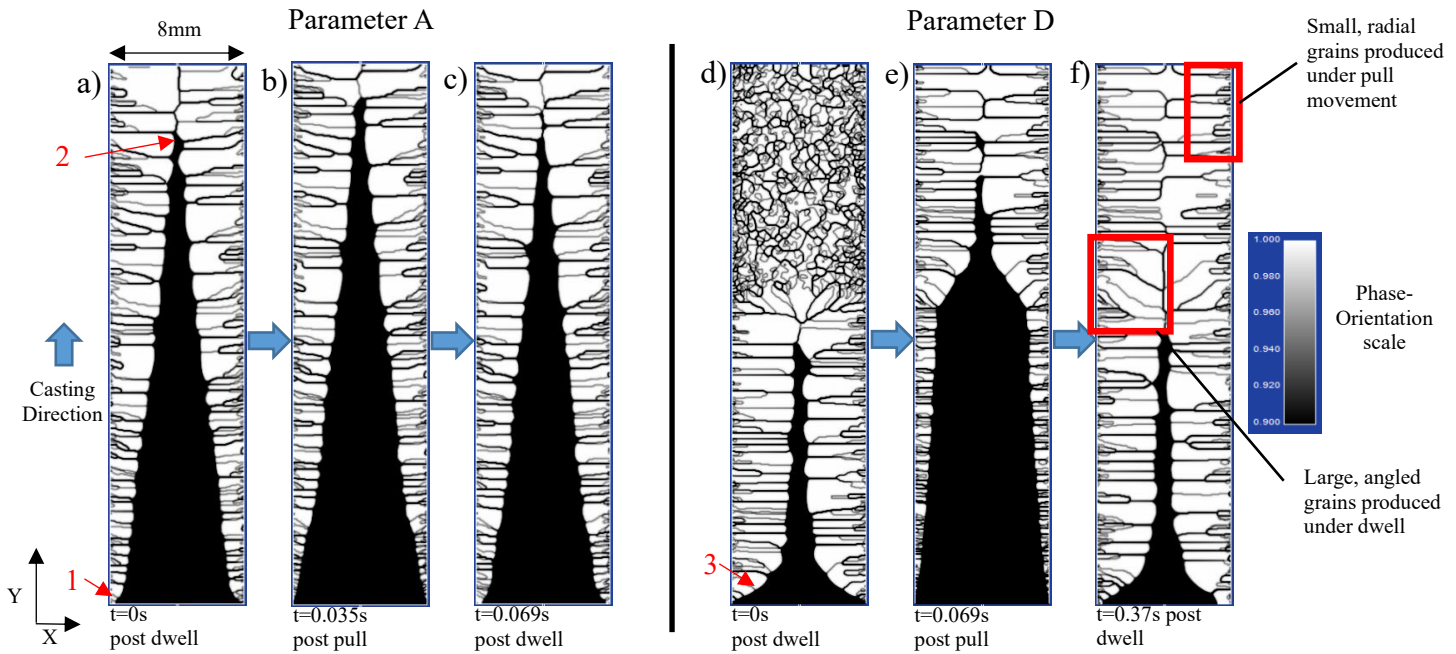


Figure 3 – Simulated transient grain growth over primary cooling zone showing a – c, Parameter A (108 kg/hr), for time frames $t = 0$ s, 0.035 s and 0.069 s respectively; and d – f, Parameter D (81 kg/hr) for time frames 0 s, 0.301 s and 0.37 s, respectively.

Figure 3 depicts 1 casting cycle for both parameter A and D, and has been arranged as follows:

1. $t = 0$ s (images a, d) image taken immediately after dwell and before pull movement
2. $t = 0.035$ s (image b) and $t = 0.069$ s (image e) immediately after pull movement, preceding second dwell
3. $t = 0.069$ s (image c) and $t = 0.37$ s (image f) similar position to $t = 0$ above although after 1 cycle.

Figure 3d shows a homogeneous grain structure towards the top of the image, this is an artefact from initial conditions.

The grain growth initiates from the outer edges of the die shown by the small white grains in the bottom corners of figure 3a. As the rod casts upwards the grains continue to grow from the edge to the center of the rod (horizontally, x-orientation) increasing in size. They grow with an angle oriented due to the heat distribution within the die [8,9] which is at a normal orientation to the heat flow, and for parameter A is perpendicular to the casting direction [13], see Fig. 4. Compared to parameter D, parameter A shows a more homogeneous solid-liquid interface. That is, an almost linear solidus front from initial solidification (point 1, figure 3a) to central solidification (point 2, figure 3a) throughout the entire cycle, with little change in fluid volume over the casting pulse cycle. Whereas, parameter A shows a significant bulge (point 3, figure 3d) in the interface which is apparent throughout the entire cycle (figure 3d-f). An inconsistent grain structure is also visible at this same point. Parameters B, C and E all produced similar grain structures and transient growth behaviours to parameter A (See figure 5).

Simulating with longer dwell durations in parameter D (highlighted in Fig.3 d-f) indicates that during the dwell

phase, the grains grow larger producing within the cast grain pattern, periodic regions of large/small grain growth (see annotations on Fig 3f). This produces a cast rod with cyclically varying mechanical properties which can be problematic for downstream processing. These larger grains also re-orient towards a parallel configuration to the casting direction (vertically in y-axis), due to the changes to the heat distribution within the casting die which is discussed in *Temperature Distribution* section.

Temperature Distribution

Parameter A has a higher throughput than parameter D (108 kg/h compared to 81 kg/h), and produces a more homogeneous grain structure as demonstrated in the *Discretization* section and in reference [8,9]. This is associated with the temperature distribution within the primary cooling zone during the withdrawal cycle, see figure 4. Temperature plots for both parameter A and parameter D are shown and highlight a variation between the two settings. This is due to the variance in average casting rate as described in the *Average temperature and solid fraction* section. The heat in parameter A protrudes, on average, 8.18mm further up the die.

The change in the grain growth direction is directly related to the distribution of heat within the die. During the shorter dwell (0.034s), the grains initiating within the lower (hottest) part of the die are less established before the next forward movement occurs. However, during the long dwell (0.301s) these grains have more time to develop, and the grain growth direction orients perpendicular to the withdrawal direction (y -axis). This is highlighted in figure 4. After the dwell, these grains then continue to grow at this angle as competitive grains from below have not yet been established to force a more radial growth direction.

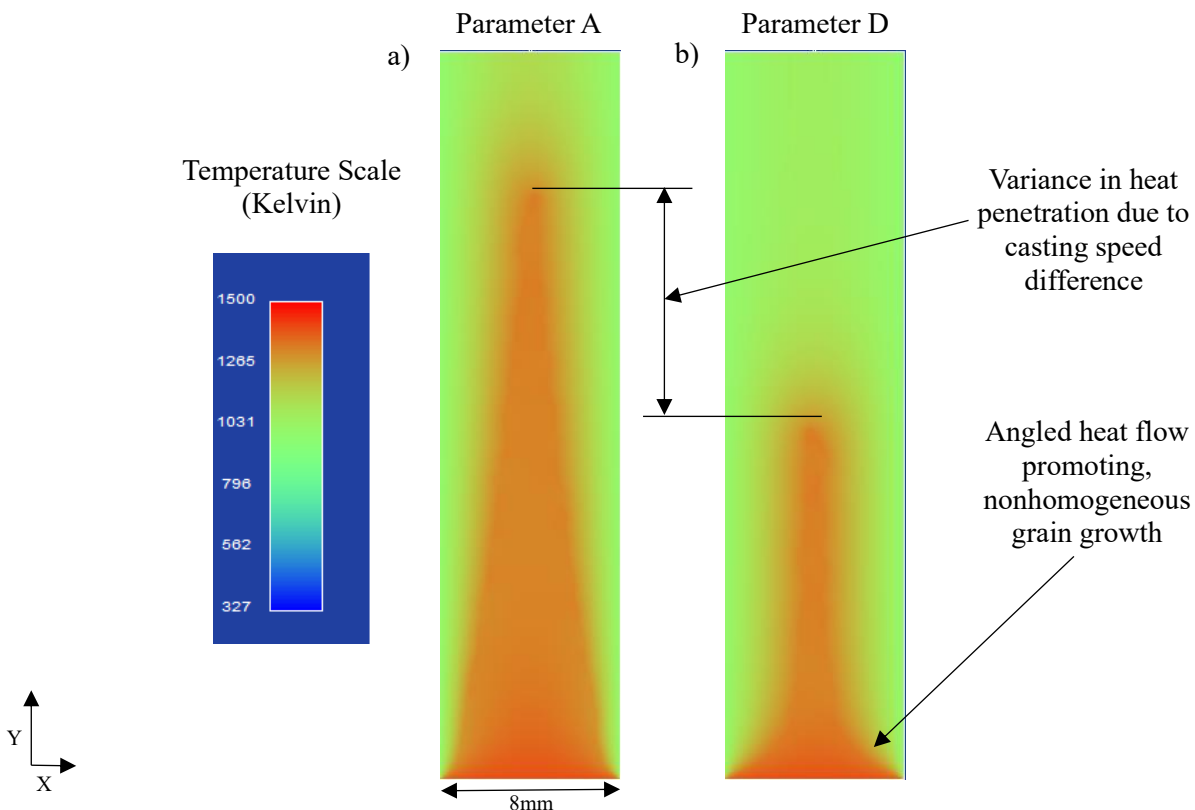


Figure 4 –a) Simulation of temperature distribution within 8 mm die primary cooling zone for Parameter A at the end of dwell period (0.035 s). b) Parameter D temperature distribution at end of dwell period (0.37 s).

Solidus Front Vertical Height

The height of the solidus front (from initial solidification to fully solidified arrow 1 figure 5) has been shown to increase linearly with casting rate in VUCC of 8mm Cu [2]. The same relationship at faster casting rates, has been observed within these simulations as shown in Fig. 5. Parameters A and B (108 and 109 kg/h, respectively, Fig.5a) have similar solidification front (SF) heights (28.3 ± 1.6 mm and 26.9 ± 1.9 mm), despite

their different pull distances and dwell durations. For slower casting speeds parameters C and E (96 and 97 kg/h, respectively), the SF heights were also similar at 23.0 ± 2.1 mm and 23.1 ± 2.5 mm, indicating that the height at which the SF protrudes up the die is dependent on the average casting rate and independent of the pull distance and dwell durations. The smallest casting rate 81 kg/h, produced the smallest central protrusion at 20.2 ± 3.6 mm. The error has been determined using standard deviation of 15 cycles for each casting setting once equilibrium had been achieved.

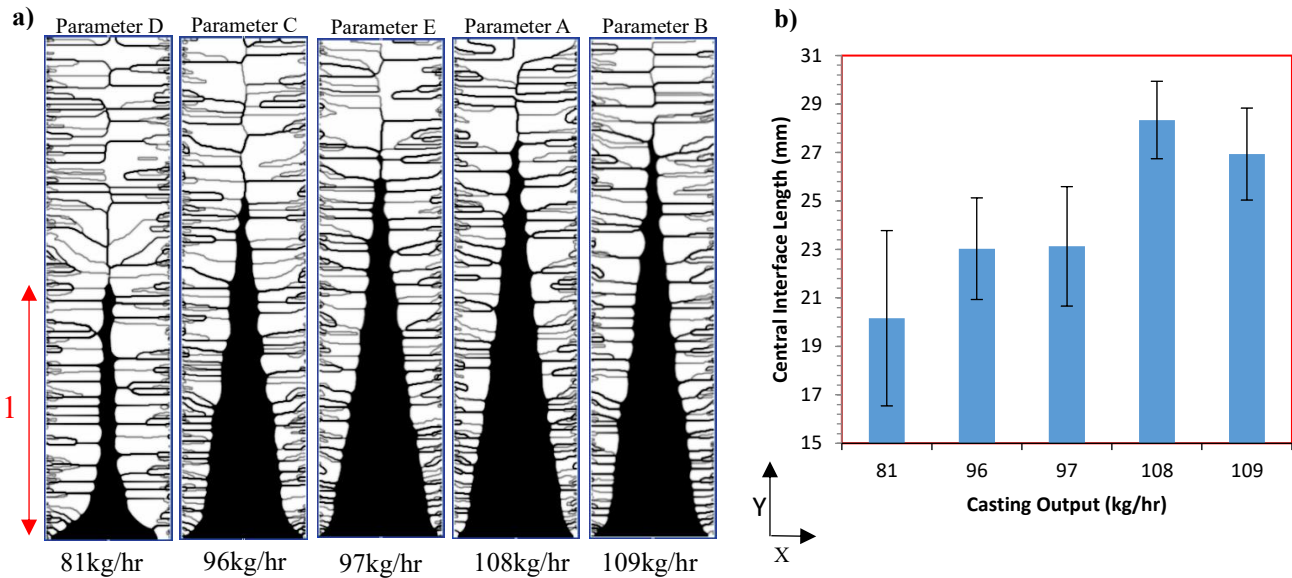


Figure 5 – a) Simulated grain structure within primary cooling zone for 8 mm die for parameters A-E, obtained before vertical withdrawal movement. b) Plot of measured average solidification front height.

Simulation validation

The simulation outcomes for parameters A & D were compared alongside their cast grain structures, shown within figure 6., to validate the observed grain structures. In a, (Parameter A) a homogeneous microstructure is cast which coincided with the simulated structure. Computational size limitations of the PhasePot™ limits the maximum computational cell size and so placing a limit on the smallest grain size resolved. For this reason, the simulated grains were not as small as their cast counterparts however, the orientations of the grain growth directions show similarities.

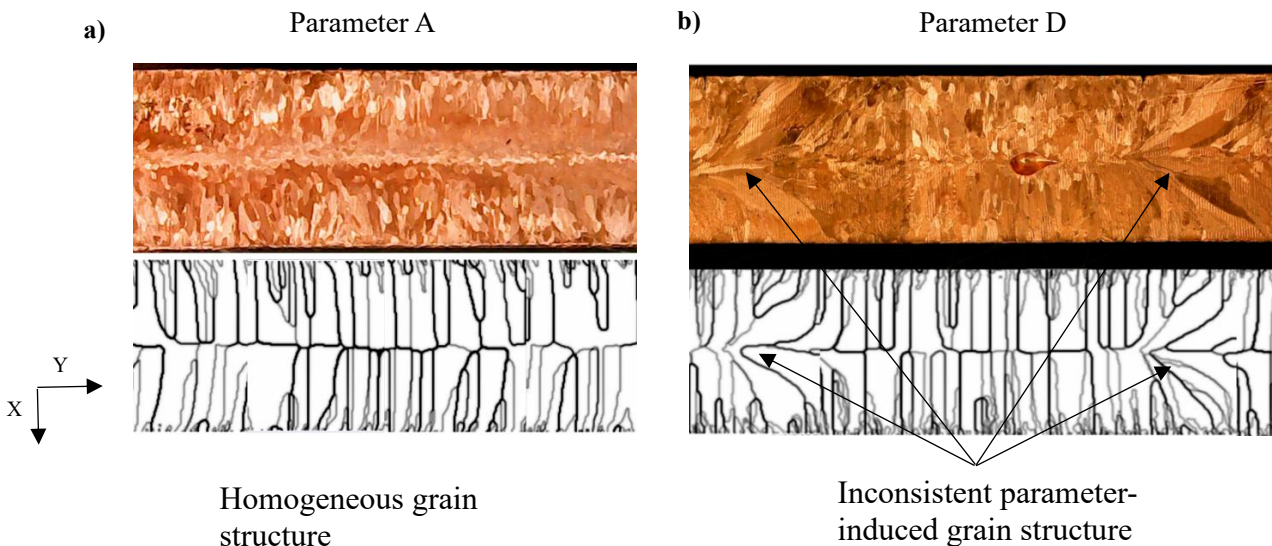


Fig.6 – a) Top, as cast 8mm copper internal microstructure from parameter A, and bottom, simulated microstructure. b) Top, as cast 8mm copper internal microstructure from parameters D and bottom, simulated microstructure of parameter D.

The simulated outcome for parameter D showed an inhomogeneous grain structure produced due to the withdrawal settings, as discussed in sections *Discretization* and *Temperature Distribution*. This inhomogeneous grain structure is also highlighted in the cast rod (Fig 6b), showing how the simulated withdrawal parameters have reproduced the casting behaviour.

Conclusion

Monte Carlo Potts coupled Phase Field simulations were used in the investigation of 8 mm VUCC cast OFCu. The source of known casting artifacts was hypothesized in a qualitative analysis between simulation and cast rod, with boundary conditions based on a previous CFD analysis for vertically continuously cast 8mm OFCu. The model was validated against cast product and demonstrated the interdependence on temperature and casting rate on the SF and the grain morphology. The presented simulation model enables prediction of grain morphology and SF which is of significance in identifying the ideal casting parameters, as well as reducing the numbers of costly casting trials required in the evaluation of said process.

REFERENCES

1. H. Soda, G. Motoyasu, A. McLean, S. D. Bagheri, and D. D. Perovic, "Continuous casting of unidirectionally solidified copper rod," *Int. J. Cast Met. Res.*, vol. 9, no. 1, pp. 37–44, May 1996.
2. K. Härkki and J. Miettinen, "Mathematical modeling of copper and brass upcasting," *Metall. Mater. Trans. B*, vol. 30, no. 1, pp. 75–98, Feb. 1999.
3. D. Mackie, J. D. Robson, P. J. Withers, and M. Turski, "Characterisation and modelling of defect formation in direct-chill cast AZ80 alloy," *Mater. Charact.*, vol. 104, pp. 116–123, 2015
4. H. R. Müller, *Continuous Casting: Proceedings of the International Conference on Continuous Casting of Non-Ferrous Metals*. Wiley, 2006 *Engineering from Tradition to Innovation*. 2015 Apr 3-5; Venice, Italy. Milan: Aim; 2016. p. 182-191.
5. I. Hadi, M.A. Jabbareh, R. Nikbakht, H. Assadi (2012): Modelling of microstructure evolution during thermal processes - A hybrid deterministic-probabilistic approach, *Materials Science Forum* 704-705, pp. 63-70.
6. W.J. Boettinger, J.A. Warren, C Beckermann, A. Karma, *Phase-Field Simulation of Solidification*, 2002, *Annual Review of Materials Research*, Volume 32, pp. 163-194
7. E.-R. Bagherian, Y. Fan, M. Cooper, B. Frame, and A. Abdolvand, "Effect of water flow rate, casting speed, alloying elements and pull distance on tensile strength, elongation percentage and microstructure of continuous cast copper alloys," *Met. Res. Technol.*, vol. 113, no. 3, p. 308, 2016.
8. T.D.A. Jones, R.I. Strachan, D.M. Mackie, M. Cooper, B. Frame, J.B. Vorstius, Optimising computational fluid dynamic conditions for simulating copper vertical casting, in: *Int. Conf. Process. Manuf. Adv. Mater.*, THERMEC, Vienna, 2021. doi:<https://doi.org/10.6084/m9.figshare.12546287.v1>
9. T.D.A. Jones, R.I. Strachan, D.M. Mackie, M. Cooper, B. Frame, J.B. Vorstius, Computational fluid dynamic simulations of solidification for enhancing speed of continuous cast copper: *Engineering science and technology, an international journal*, 2021-02, Vol.24 (1),p.92-104. doi:10.1016/j.jestch.2020.12.009.
10. L. Nastac, K. Pericleous, A. S. Sabau, L. Zhang, and B. G. Thomas, *CFD Modeling and Simulation in Materials Processing 2018*. Springer International Publishing, 2018.
11. "ASTM International, ASTM E112-13, Standard Test Methods for Determining Average Grain Size," 2013
12. Phasepot, *Microstructure Development Studio Phasepot 1.0 User's Guide*, 2014
13. PORTER, D. A., EASTERLING, K. E., & SHERIF, M. Y. (2009). *Phase transformations in metals and alloys*. D