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The Modelling Of Oxide Film Entrainment In Casting Systems Using Computational Modelling

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Abstract

As Campbell stated in 2006, "*the use of entrainment models to optimise filling systems designs for castings has huge commercial potential that has so far being neglected by modellers*". In this paper a methodology using computational modelling to define entraining events and track the entrained oxide films is presented. Research has shown that these oxide films present within the casting volume are highly detrimental to casting integrity, thus their entrainment during mould filling is especially undesirable.

The method developed for the modelling of oxide entrainment has been validated against previously published data by Green and Campbell (1994). The validation shows good quantitative correlation with experimental data. However there is scope for further development which has the potential to both improve the accuracy and further validate the technique.

Introduction

Minimising development costs and time is now essential to stay competitive in the foundry industry [1]. Therefore computational modelling is now seen as a necessity to give rapid and cost effective product development. This has been further aided by the development of commercially available optimisation software to replace the current qualitative techniques used by the foundry engineer to design casting running systems.

A single quantitative value is required by optimisation software to use as a goal. Kokot and Burnbeck [2] have given an overview of the current state of the optimisation software. The use of optimisation tools has lead to the topic of quantification of oxide entrainment to be of upmost importance for both industry and software companies. Indeed Kokot *et al.* [3] stated that optimisation can only be *"obtained if the right quantitative criteria to formulate the objective functions are available"*. These quantitative criteria for casting integrity still require development. Campbell stated that "*the use of entrainment models to optimise filling systems designs for castings has huge commercial potential that has so far being neglected by modellers*" [4].

Due to the importance of entrainment in the casting process and other applications there have been a number of attempts at developing models to predict and often quantify this entrainment. Historically a

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variety of different solutions with differing methods, abilities and benefits have been developed to quantify oxide entrainment, as largely summarised by Campbell [4] and critically reviewed by Reilly *et al*.[5] . The modelling of entrainment can largely be broken into two categories, the modelling of indiscrete and discrete defects. Indiscrete defect modelling is defined as models where the magnitude of the total amount entrained defects may be either quantitatively or qualitatively assesses but the location of each individual defect is unknown. This type of model is often computationally more efficient than the modelling of discrete defects. Below, a summary of the significant defect modelling techniques is given.

One of the simplest methods for indiscreetly modelling defects is the assessment of the free surface area as undertaken by Lai *et al*. [6-7] and Sun *et al*. [8]. The work by Lai *et al.* compares the modelled instantaneous free surface area against the minimum free surface area expected if the mould had filled in a perfectly tranquil manner. The greater the difference between these two values, the larger the excess of free surface area, the greater the likely magnitude of free surface entrainment. The major limitation of this methodology is the calculation of the expected free surface area should the mould have filled in a perfectly tranquil manner. For all but the simplest geometry this is extremely challenging to calculate. However, the comparison of the excess free surface area for castings of identical geometry allows direct comparison and thus potential optimisation. Sun *et al.* report positive results using this technique in an industrial environment.

Methodologies based around dimensionless numbers have been published; these are commonly based around the Froude (ratio of inertial to gravitational pressures) or Weber (ratio of inertial to surface tension pressures) number [9-13] . These models commonly focus upon discrete locations within the model, for example the casting in-gate or runner bar, and thus can only partly describe the entrainment within the casting system.

Cumulative scalar techniques have been developed by multiple software developers [14-16]. These techniques place a scalar value upon the liquid free surface to describe the growth of oxide upon the melt surface. This scalar is allowed to diffuse and advect throughout the liquid. The rate of scalar accumulation is described as a constant growth rate. The scalar represents the likely hood of defects being present. This technique is probably the most widely use entrainment defect prediction tool in the casting industry.

As stated by the Barkhudarov and Hirt [15], the cumulative scalar technique does have some drawbacks in the casting scenario, namely:

- The adhesion of oxide film to mould walls is not accounted for.
- No oxide film strength is modelled
- No buoyancy of oxide film is modelled
- Without any experimental results the significance of the absolute values of the scalar are meaningless. However the defect location patterns are still valid.

Many of the other techniques described here also suffer from one or more of the above drawbacks, they are not limited to the cumulative scalar technique.

Blair *et al.* developed a discrete defect tracking method based upon the growth of discrete particles when they are upon the liquid free surface. The technique is aimed at modelling re-oxidization inclusions in steel. Particles of negligible size are placed in the liquid, when these particles are upon the free surface they grow at a defined rate, this represents their oxidisation. The particles size, mass and advection are modelled. The agglomeration of particles is allowed. The final location of the particles after solidification has shown good agreement with experimental data obtained in industrial settings [17-18].

Work by Ohnaka *et al.* used a methodology similar to that presented in this manuscript. This manuscript further develops and also experimentally validates this technique. Ohnaka *et al.* used Boolean logic criteria to predict entrainment, representing the defect by a particle who's advection is modelled [19]. This technique initially modelled bubble entrainment and porosity before being extended to oxide film entrainment [20-21].

This manuscript presents a methodology for modelling free surface entrainment using computational fluid dynamics. The methodology uses Boolean logic criteria to assess if free surface entrainment has occurred, if entrainment is found particles are used to mark the entrained surface film. The motion of the particles is simulated in order to obtain the final defect location. The work has been validated against experimental data obtained from the casting of aluminium A356 samples. The integrity of these samples has been characterised by the Weibull modulus [22], obtained from tensile test data. This study has been focused on aluminium casting and the modelling of the oxide film present upon the melt surface. However, the same methodology could easily be applied to other casting material with surface films, such as iron or steel, and other fluid flow scenarios where entrainment of the free surface within the bulk liquid is of interest.

Methodology

A user customisation to the commercial CFD (computational fluid dynamics) software Flow-3D, Oxide Film Entrainment Model (OFEM), has been developed to allow the assessment of entraining events and the marking and tracking of entrained oxide films. This allows the final defect location(s) to be identified. The OFEM has been developed such that it is capable of interrogating the full 3D free surface.

Flow-3D version 9.3.2 was the CFD (Computational Fluid Dynamics) used in this work. A brief description of this software follows, further information on the techniques described here can be found on the Flow-3D website [23] via the Technical Notes and CFD-101 web pages or in the Flow-3D user manual [24].

The software uses a structured Cartesian mesh, either a single or multiple mesh blocks can be utilised in a model. Any mesh block can be manipulated to allow cells of different aspect ratios to be present within a single mesh block. This allows the user the opportunity to improve the definition of geometry within a specific region of the model without generating and excessive numbers of cells, which would in turn produce long simulation times. Inserting a fine mesh block within the volume of a coarser one also allows the improved localised definition of geometry whilst maintaining respectable simulation times.

The software exclusively uses the Fractional Area Volume Obstacle Representation (FAVOR) [25] technique to define geometric obstacles within the Cartesian mesh. This technique allows Flow-3D to utilise simple and efficient Cartesian grids to define complex geometrical shapes. FAVOR works by blocking out both whole and fractional portions of grid cell faces and volumes. The meshes used in this paper were all regular (sides of equal length) Cartesian meshes of 1.25 mm. This gave model of approximately four million mesh cells, resulting in runtimes of 672 hours (4 weeks).

Free Surface Tracking - the software uses the Volume of Fluid (VOF) technique to model fluids with free surfaces. This technique was first developed by Flow-3D's founders Hirt and Nichols [26-27]. VOF consists of three elements; a methodology to locate the free surface, an algorithm allowing the tracking of free surface as a sharp interface as it moves through the computational mesh and a method of allowing boundary conditions to be applied at the free surface

The fraction of fluid (1 = fluid region, 0 = void region) both present within a cell and present within neighbouring cells is used to define the free surface. A detailed description of the methodologies employed by VOF has been given by Barkhudarov [28]. Flow-3D incorporates a number of turbulence models in this case the Renormalized Group k-ε turbulence model (RNG) [29] was used as the flows were expected to be highly turbulent.

Below is a summary of the OFEM, a full description can be found [30].

Defining entrainment events - Each cell within the Cartesian mesh domain has a single value for each physical property, for example; velocity (in each axial direction), density, temperature, fraction solid, open fraction, fraction of fluid, *etc.* Each cell has a free surface Normal Front Value (NF Value). This is the primary normal direction to the free surface. This value also defines cells which have no free surface, *i.e.* cells with a fluid fraction of one or zero.

Each cell in the meshed domain is scanned. If the cell has a free surface and has not had a particle placed within a user defined time period then the cell is assessed against the entrainment logic. Using the NF values, velocity values, fractions of fluid, free surface area, fluid fraction at beginning of cycle and fluid fraction at the end of cycle, a series of Boolean logic criteria were defined to determine the occurrence of entraining events. An example can be seen in Figure 1 a) where the Boolean logic criteria for a plunging jet is schematically depicted. If the free surface normal values (NF values) in the respective cells are as shown, and the velocity vectors are converging then an entraining event is deemed to have occurred. Figure 1 b) shows a schematic for a colliding free surfaces entrainment case in the YZ plane. It would be expected that the collision of fluid fronts would require the logic that two neighbouring cells have opposing NF values and a fluid fraction of less than 1 at the start of the cycle and 1 at the end of the cycle. However, the way in which Flow-3D is programmed means that this logic is not a working solution for this particular software. Implementation in Flow-3D requires the logic of an interior cell (NF = 0) but with a free surface value greater than 0 (a combination which logically should not be able to exist) and with a fluid fraction of less than 1 at the start of the cycle and equal to 1 at the end of the cycle must be found to indicate a colliding front. The free surface values is a scalar calculated by the Flow-3D software and available as a sub-routing variable. The plane upon which this free surface collision is occurring is determined by assessing the NF values of the surrounding cells.

The Boolean logic criteria used allows entraining events to be defined in all planes, giving a full 3D implementation of the entrainment model.

Placing Particles - When an entraining event has been identified a particle is placed within the assessed cell to represent the entrained oxide. The particle model within the software was used, with the initiation location and velocity vector being calculated by the user customisation. Each particle added was given a density and size corresponding approximately to that of an oxide film. Particles must be of either of the same size, but varying in density or of the same density but varying in size. The coefficient of restitution for all particles was also identical for all particles within the domain. They can either stick to the mould wall indefinitely upon impact or be reflected from the mould wall with a fractional energy loss of factor 1 (keeping all its energy) to 0 (sticking to the wall but being able to be scoured from it). Using a negative number for the coefficient of restitution creates particles which will stick to the mould wall indefinitely. It was not possible to assign different properties to each particle to be more representative of oxide films where each is unique. The particles were placed in the most representative location within the assessed cell.

Once a particle had been placed, the time period of placement was recorded as a scalar for that cell. In every time period this scalar was assessed. Once the scalar was less than the current time period

minus a user defined value the cell was once again assessed for entraining events. This allowed the user to regulate the frequency of particle placements within a given cell to stop over-population of particles. This also limited the effect that the simulation time step had on the number of particles placed. This has the effect of taking into account the finite (although very small) time it takes for oxide films to form.

Data Output - The number of each entrainment type, frequency of entrainment in each mesh block, number of particles placed and present in each mesh block and the number of particles both entrained and present in user defined regions were recorded and output into text files.

Validation Of Oxide Film Entrainment Model (OFEM)

Initial validation of this model was undertaken using work published by Green and Campbell [31]. The running system modelled both with and without a 10 ppi reticulated foam filter is described in Figure 2.

Model input parameters are summarised in Table 1and fully defined [30]. For models using a filter the properties used are those defined by Lo [32] and are described in Table 1. Further information on the methodology used, an equivalent pressure drop method, to model flow through the filter can be found in the software user manual [33] and [32, 34].

The experiments were simulated as accurately as possible with the data available from the published paper by Green and Campbell [31]. This did not allow the modelling of the pour as they were hand poured and the parameters were not available.

A pressure boundary was used for the inlet condition. For the inlet a falling stream of circular cross section was positioned to impact centrally the bottom of the pour basin after falling vertically. It was believed this gave, as closely as is possible, a realistic representation of a hand pour. The diameter of the inlet was 36 mm. The stream was a representation of pour being initiated 25 mm above the model (pressure boundary of 550 Pa applied) in addition to the 50 mm of free fall the stream experienced within the model domain. This allows for a rapid initial filling as characteristic of manual pours. After 0.65s, the pouring basin is almost full and the flow rate of metal in the pouring stream is reduced to replicate the action of the caster in hand pouring. This was achieved by using a moving object that covers most of the inlet at 0.65s. The models were simulated with both flow fields and thermal fields modelled until solidification of the test specimens. This allowed the final defects' (particles') locations to be determined.

The size of the particles added to the flow was defined by assuming that the defects were thin films with a layer of entrapped air between the two oxides. From past work oxide films have been commonly measured at 0.5 – 2.0 mm in length [31, 35-38] although both much larger and smaller films have been identified in published works [39-40]. Based upon the published data a maximum and minimum square defect size was defined wherein the maximum and minimum side lengths of a square defect were 2 and 0.5 mm respectively, and the thickness of the defect one tenth of the square edge length. The defect volume was then translated into an equivalent sphere diameter that could be specified as the particle diameter within the model.

The spherical particles were sized randomly between 25 and 31 μm diameter. Oxide films are individually unique, varying in size, shape and density. However, due to the limitations of the

software it was not possible to give each particle a unique size, shape and density. A particle density of 2250 kgm^{-3} was assigned assuming that each double oxide film had been created with a small volume of entrapped mould gas (air). Therefore, the overall density of the defect was lower than that of the surrounding fluid, even though the density of aluminium oxide is greater than that of aluminium [37].

Work has also shown that when a filter is used there is the possibility of the oxide films becoming shredded and thus become more numerous and smaller [41]. This was not accounted for in the model.

A simple model was used to assess the sensitivity of the software particle model to both particle density and size [30]. The model used had low velocity flow fields, thus it was felt that it would be more sensitive to particle characteristics. The study showed that the particle motion is affected when the density and/or sizes of particles are dramatically changed. These results showed that there is negligible difference in particle motion for particles of this scale. Only at scales an order of magnitude greater were any noticeable effects seen, however these were still small. It appears that the density has negligible effect. Differing orders of magnitudes were not assessed for density as it was felt that these values would fall outside of reasonable values for the density of oxide films. It is expected that the density parameter become less sensitive as particle diameter is decreased, due to the buoyancy effects becoming smaller. Although the methods used to define particle properties may appear crude it has been shown in sensitivity studies that the strong velocity fields encountered during casting will mean that particle size will have a negligible effect so long as the order of magnitude is correct.

It has been suggested that that for particles less ≤ 0.05 μm (approximately) there is a fundamental problem in simulating their behaviour in fluid flows. This is because the boundary layer thickness developed on the particles surface becomes greater than their own size. The Navier-Stokes and Lagrangian equations are therefore no longer applicable [42]. Only current work by Griffith *et al.* [43-44] has allowed the possibility of accurately assessing a simulation software particle tracking model. It is obvious that further work is required to further refine the particle characteristics to be used in the OFEM.

A user customisation was written to count the number of particles within the gauge length of the test bars (central 40 mm portion of the test specimen). Data from this sub-routine were written into a text file at a user defined frequency of 100 Hz.

A second user customisation was written to count the number of entraining events that occurred within a user defined area. Both the total number of entraining events and entraining events caused by plunging jets in both the pour basin and filter print volume were counted.

Results

Experimental results

The published data by Green and Campbell gives a Weibull modulus [22] of 19.7 and 37.7 for the non-filtered and filtered conditions respectively [31]. Previously unpublished experimental data by Green is shown in Figure 3. These data are from a mould which is different to that used for both the modelling and experimental results. It is a modified version of that described in Figure 2. The modifications are the runner depth, which has been increased in the real-time X-ray data along with the geometry of the filter print the runner bar junction. This can be clearly seen in Figure 4. Even

though the mould geometry is different it is possible to compare the model and real time X-ray data for the period of the initial filling of the filter print as the geometry changes have no effect.

The real time x-ray results correlate well with the model (Figure 5 and Figure 6), showing the same flow patterns. The unfiltered condition shows an initial folding of the fluid surface onto itself (Figure 3, 0.16 s to 0.32 s), followed by a persistent entraining plunging jet (Figure 3, 0.48 s to 0.80 s). The filtered condition shows the filter to suppress the entraining flow mechanisms of plunging jets and folding surfaces.

Modelled Results

The results of the simulations can be seen in Figure 5 and Figure 6. These show that there is large-scale entrainment in the pouring basin from both the initial turbulent filling and the subsequent persistent plunging jet. The turbulence within the basin disperses the particles throughout the bulk liquid. With the exception of the filter print in the unfiltered system there is very little further entrainment due to a well designed running system. In the filter print of the unfiltered system a second persistent plunging jet is formed by the fluid stream from the down-sprue exit impinging into the volume of fluid in the partially filled filter print (Figure 7). This caused further entrainment of oxides into the already damaged fluid.

The data for the number of entraining events recorded in the filter print and pour basin, alongside the number of entraining events deemed to be from plunging jets in both the pour basin and filter print, can be seen in Figure 8. These show the greatest proportion of entraining events in both the pour basin and filter print to be largely made up of entrainment caused by plunging jets.

It can be seen that the initial stream of metal contains the highest density of particles. This is due to the extremely high level of entrainment experienced by the initial metal stream impinging on the bottom of the basin and then rolling over as the fluid hits the side walls of the basin. This initial metal stream eventually ends up in the outer test bars (test bars 1, 2, 9 and 10). This causes the uneven distribution of particles as seen in Figure 9. It can be seen in Figure 9 how the distribution of particles in the test bars varied depending on the filter condition. However the general distribution still suggests that the outer test bars should be of lower integrity than those closest to the down-sprue.

Discussion

The modelled results agreed with those found experimentally, although further data are required for full validation. The filtered condition, which was shown experimentally to be of greater integrity (Weibull modulus 37.7), had an average 1458 particles in the gauge length, compared to an average of 1945 particles for the unfiltered condition (Weibull modulus of 19.7). It is realised that the filtered results appear to show more scatter in the data, however it must be remembered that many of the test bars from the unfiltered conditions were not able to be tested. If these are taken into account then the scatter for the unfiltered conditions becomes much greater than that of the filtered conditions. This suggests that this technique is appropriate for quantifying free surface entrainment. However further investigations to give a much larger data set and using a variety of running system designs which emphasise different entraining flow phenomena are required for this to be conclusive.

The experimental results show the defects “easily identified as oxides” [31] to be the failure mechanism of the test samples. Therefore it is known that the failure mechanism is due to the entrainment mechanisms modelled by the OFEM rather than another unaccounted for factor.

The inclusion of the pouring basin and its persistent plunging jet in the model entrained large numbers of particles which remained in the bulk and travelled through to the test bars. High levels of turbulence were present within the basin which distributes the entrained oxide throughout the fluid. It has been shown previously that pouring into a basin is likely to be the most entraining portion of the whole filling of a mould [7]. However, this work [7] suggested that this was due to splashing and folding of the fluid surface . These results show that it is due to a persistent plunging jet. The results described in Figure 10 show how the persistent plunging jet accounts for 61 – 68 % of the entraining events recorded in the pouring basin. Thus it is the plunging jet rather than the folding and splashing of the fluid surface which causes the majority of oxide film entrainment. However, it must be remembered that although the OFEM does define and track entraining events it currently does not quantify the amount of entrained oxide. It is incorrect to assume that the number of particles directly correlates with the number of oxide films which would be created experimentally from the same flow phenomena. The area or quantity of oxide film entrained at a plunging jet is dependent on the velocity of the stream impinging on the fluid alongside the state of the fluid it is impinging into (including surface undulations and bulk flow fields). This is not quantified by the OFEM. The folding and splashing of a free surface is largely modelled by the collision of two fluid fronts. This means the area of entrained oxide film represented by each particle is approximately equal to the mesh size. Therefore the area of entrained oxide film will be different for the different entrainment mechanisms, meaning that it is not possible to categorically state that the number of particles entrained correlates with the area of oxide film entrained and thus damage to the material. It is anticipated that future development of the code can define the particle size as a function of the area of entrained oxide film.

The extremely damaging nature of the plunging jet is shown by Ohl *et al*. [45] who found that perturbed streams, of which the stream of fluid flowing from the crucible almost certainly is, falling into a volume of liquid is generally entraining. This work by Ohl *et al.* showed that for a perfectly smooth liquid stream (something obviously extremely difficult to produce in a transient casting process) no entrainment will occur. Entrainment is only initiated when there is a surface perturbation. This is independent of fluid height. Although work on pour basin design [46] has been undertaken no studies have been conducted into the effect the pour characteristics, such as height of pour, steadiness of the crucible or flow rate have on casting quality. The predominant entrainment mechanism in these models is the plunging jet (Figure 10). Further validation against data with different entrainment mechanisms would be beneficial. However, no published data which is of suitable detail and clarity is available

The initial melt material can be seen to contain the highest density of particles (Figure 5 and Figure 6). This material finally resides in the outer test bars giving the skew to the results seen in Figure 9. This result is further evidence to add to the findings of Campbell [47] that a correctly designed overflow to capture the initial metal stream and dissipate energy is beneficial to casting integrity.

The experimental results from Green and Campbell [31] showed the filtered data to have a much smaller spread of properties when compared the unfiltered condition. This is shown by the standard deviation of the filtered and unfiltered condition strengths being 9.34 and 14.66 respectively. A comparison of the modelled results shows a much wider spread of normalised results (fraction of largest value encountered). This ranges from 0.26 – 1 for the modelled data in comparison to 0.79 - 1 for the experimental data.

The average number of particles was seen to be greater in the gauge length of the unfiltered castings when compared to that of the filtered conditions. The modelled conditions have standard deviations of 655 (mean of 1458 particles) and 652 (mean of 1945 particles) for the filtered and unfiltered conditions respectively. Although the magnitude of these cannot be compared directly to that of the experimental data, it is noticeable that the standard deviations are approximately the same as each other, as compared to the experimental data which show a marked difference. This could be interpreted as the model suggesting that the data sets for both modelled conditions should have a similar spread of results, clustered however around a different tensile strength (TS). The reduced number of particles in the filtered condition does correlate with the increased TS shown by the filtered condition experimental data. However, the spread of results modelled using the OFEM was seen to be greater for the filtered conditions than the unfiltered ones. This suggests a greater variation of mechanical properties for the filtered condition. This was not supported by the experimental evidence, which gave a greater Weibull modulus to the experimental results of the filtered condition (19.7 compared to 37.7 for the unfiltered and filtered conditions respectively). Thus the filtered condition to have both, a higher TS and more consistent mechanical properties. These results obtained in this research indicate that the OFEM is correctly modelling entrainment of oxide into the bulk fluid but is not be modelling their transport and life (events occurring to the oxide films) correctly. Possible reasons for this will be later described. It must also be remembered that it is the most damaging defect which dictates the TS rather than the number of defects. Obviously the larger the number of defects, the more likely a larger and more damaging defect will be present.

The Weibull statistical technique [22] was used to analyse the inverse number of particles in the gauge length of each test bar Figure 11. This gave the Weibull modulus of 20.0 and 27.5 for the unfiltered and filtered conditions respectively. This shows agreement with the experimental data of Green and Campbell (19.7 and 37.7 for the unfiltered and filtered conditions respectively). It should not be expected that the Weibull numbers should be the same as the experimental and modelled and results are of different data types (tensile strength and the reciprocal of the number of particles respectively). However, it should be noted that both sets of data suggests that for the filtered condition, both the reliability and the average value is increased when compared o the unfiltered condition.

It is not possible to reconcile the experimental strength data to individual tensile test specimens and it is unfortunately not possible to determine if the strength results match the clear pattern suggested by the modelled results in Figure 9. Here the outer test bars are shown to contain more defects when compared to the centrally located ones. However, in a study of the fatigue life distributions of Al-7Si-Mg alloys cast through very similar (but not identical) running systems [48], the fatigue lives of the outer bars were consistently lower than those of the inner bars. Failure of the outer bars was normally initiated by oxide film defects.

The incorporation and transport of particles within the liquid metal as reported in this paper is not unique. Algorithms for doing so having been described previously by Yang *et al.* [49-50] and Ohnaka *et al.* [19]. It is considered that this method is an improvement on the Yang method as it is implemented in three dimensions, can assess all entrainment mechanisms and identify them individually. It is an improvement on both methodologies as it is the only code thus far to be targeted at optimisation, and thus incorporates quantitative assessment techniques of the final particle locations.

There are limitations for the accuracy of this technique which require further development and understanding, namely:

Oxide films are individually unique, varying in size, shape and density with a much higher aspect ratio than the particles actually modelled. However due to the limitations of the particle model it is not possible to assign to each particle a unique size, shape and density. In the low energy flow fields found in the test bars between filling of the mould and solidification, the buoyancy and drag force of each particle will determine their final position. The use of spherical particles of the properties prescribed in this investigation to represent individually unique oxide films is currently not able to be validated due to the lack of experimental data.

The model does not allow particles to interact. To date no experimental work has been published into the adhesion of oxide films to one another. However, it is possible to interpret the networks of highly tangled oxide films [37] and large dross defects [51] in published work as evidence for the scenario that oxide films adhere to one another should two films collide. Further detailed investigations are required to confirm this hypothesis. Work by Carlson *et al.* [51] (dealing with re-oxidation rather than oxide film inclusions) allowed particles to agglomerate as a way of easing the computational load. This was modelled after some investigation into inclusion locations which suggested (although not conclusively) that re-oxidisation inclusions agglomerate [51].Experimental work has shown that when a filter is used there is the possibility of the oxide films becoming shredded, thus becoming more numerous and smaller [41], although this work is not conclusive. It is possible that the defect sizes different for both cases. It could be speculated that defects coming from the pouring basin and down-sprue may end up smaller and more numerous in the filtered case than of the unfiltered case because the filter may shred the oxide films, as previously described. Moreover the severity of the entrainment event in the filter would be expected to be lower, thus potentially leading to less numerous and smaller oxide films.Currently this is not accounted for in the model.

The changing of the oxide morphology (for example a large thin film becoming ‘screwed up’ into a ball) between its formation and its final form in the solidified material. The morphology of the particle will have an effect on its drag force and thus motion. This has not been accounted for in the model.

The filter model used in this investigation removes the fractional proportion of particles equal to that of the closed fraction of this filter. In this case the filter removes 27.6% of particles passing through it as the software automatically removes a fraction of particles equal to the closed area fraction of the specified filter. The accuracy of this is unknown.

The actual flow through a filter and the potential damaging effect on the metal quality is not simulated here. This damage is caused by multiple fluid streams being created during the passage through the filter before, before merging once out of the filter. This is obviously only occurs in the priming of the filter which is short in persistence. Instead a pressure drop method is used to represent the filter. This is due to the severe computational penalty of simulation flow through a filter as was clearly shown by Jolly and Gebelin [52].

The accuracy of the particle model is unknown. Current work by Griffiths *et al* [43-44] has allowed the possibility of accurately assessing a simulation software particle tracking model. Currently the particle-fluid coupling has only been assessed qualitatively [53].

The models were simulated as accurately as possible with the data available from the published paper [31]. This did not allow the modelling of the pour as no data were available. This is unfortunate as unpublished work at The University of Birmingham has shown the pour conditions to greatly impact the fluid flow within the mould, both experimentally and in simulations.

The 40 mm by 12 mm diameter gauge length of the test bars was used as the volume to assess the total number of particles. However the experimental results were taken from the machined gauge length (40 mm by 6.75 mm diameter) which is obviously a source of error. It was not possible to assess the number of particles in this same region in the computational model as Flow-3D uses a Cartesian mesh which is therefore unable to define the circular 6.75 mm cross section without being extremely fine and thus computationally very intensive. As seen in Figure 11 the particles appear to be randomly distributed throughout the gauge length. This suggests that although not removing the excess volume from the bars (as done experimentally by machining) will make a difference to the quantity of particles, it is unlikely to change the rankings of the results. During machining 70.6 % of the material volume is removed from the gauge length of the test bars.

The coefficient of restitution used in the models determines that particles lose all their energy upon contact with a wall and stick to it. However, if the fluid has enough energy they can be scoured from the wall and re-enter the flow fields. Alternatively the films may not attach to the external casting surfaces. There has been no research into the adhesion of oxide films to mould walls, therefore this assumption has no experimental validation.

As can be seen many of the above areas for development require extensive experimental work to allow the correct physical phenomena to be modelled. In many areas it is the lack of real world data which hinder the modeller rather than the technicalities of the modelling itself.

Conclusions

1. The modelling of entrainment defects and quantitative assessment of casting integrity is of significant importance to the foundry industry, especially with the commercial availability of computational optimisation software.
2. A method has been presented here which uses Boolean logic criteria to define entraining events and then places particles to track them. This initial validation shows the technique to correctly distinguish casting integrity between two differing running systems.
3. Improvement over previous models as it is implemented fully in three dimensions. This method can assess all entrainment mechanisms and identify them individually
4. This is also the only code thus far to be targeted at optimisation, and thus incorporates quantitative assessment techniques of the final particle locations allowing a single quantitative number to be obtained to characterise the casting integrity. This makes the technique valuable for use in optimisation software as these require a single numeric value for which to optimise the model to. Previous techniques have relied on engineers qualitative interpretation of the model data.

5. There are still many aspects of this model which can be further developed. This will require both modelling and extensive experimental investigations.

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	Property	Value
Particle Properties	Particle type	Variable diameter
	Particle density	2250 kg m^3
	Free surface interaction	Particles move in fluid only
	Minimum particle diameter	0.00002500 m
	Maximum particle diameter	0.00003125 m
Filter Properties	Porosity model	Active
	Porous fraction [32, 34]	0.724
	Drag coefficient A [32, 34]	28.95
	Drag coefficient B [32, 34]	6.203
	Heat transfer to fluid [54]	20,000 Wm^2
	Heat transfer to void [55]	34 Wm^2
	Thermal conductivity [54]	10.9 $Wm^{-1}K^{-1}$
	Initial temperature	298 K
	Density x spec. heat [54]	1.8 e^6
Mold Properties	Heat transfer to fluid	1500 Wm^2
	Heat transfer to void [55]	34 Wm^2
	Thermal conductivity [56]	0.65 $Wm^{-1}K^{-1}$
	Initial temperature	298 K
	Density x spec. heat [56]	1500240
Fluid Properties	Density (liquid) [57]	2392 kg m^{-3}
	Density (solid) [57]	2680 kg m^{-3}
	Viscosity [57]	0.00119 Pa s
	Surface Tension [57]	1.117 N m^{-1}

	Contact angle	160 °
	Solidus temperature [57]	823 K
	Liquidus temperature [57]	888 K
	Latent heat of fusion [57]	4.29 e^5
	Heat transfer to void [55]	34 Wm^2
	Specific heat [57]	1190 J kg^{-1} K^{-1}
	Thermal conductivity (liquid) [57]	67.9 W m^{-1} K^{-1}
	Thermal conductivity (solid) [57]	145 W m^{-1} K^{-1}
	Thermal expansion [57]	-0.212
	Surface tension coefficient [57]	1.117 N m^{-1}
Miscellaneous	Contact angle	160 °
	Heat transfer model	Active
	Viscosity options	Newtonian viscosity
	Turbulence model	Renormalised group model (RNG)
	Mesh size	Uniform cubic mesh of sides 1.25 mm

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