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The Present State Of Modeling Entrainment Defects In The Shape Casting Process

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Abstract

The entrainment of oxide films into the bulk material has been shown to have a detrimental effect on casting integrity. A number of mechanisms have been shown to initiate the entrainment of oxide films, including: returning waves, plunging jets, bubble trails and fountains. Therefore, the assessment of the casting system for these features by the foundry engineer is critical in improving casting quality.

The use of computational fluid dynamics software packages, which are now widely available to the foundry engineer, has allowed the foundry engineer to improve casting system design by using qualitative parameters. Optimization software is now an economically viable option for many foundries. However, optimization for casting integrity requires a quantitative casting integrity assessment technique, which allows the modeling and quantification of defects. Therefore, modeling and quantification of defects is becoming an ever more important research area to allow the optimization software manufacturers to meet the needs of industry.

The current methods found in published literature for the modeling of casting defects have been described and critically reviewed, shedding light on the qualities and issues currently associated with the present available methods. However it is clear that further investigations and developments are still required to allow the accurate and efficient modeling of casting defects. The topics of research relating to the modelling of casting defects which require further investigation have been highlighted.

Introduction

With competition within the foundry industry becoming fiercer and customers demanding higher quality components, shorter development times and more complex geometry, the use of computational simulation has become essential to stay competitive [1]. In recent times the economic viability and increased ease of use has encouraged many larger foundries to use computational optimization software. The modeling of defects is essential to allow the optimization of casting systems for component integrity. Optimization can only occur if "*the right optimization criteria to formulate the objective functions are available"* [2]. Therefore, to optimise a casting system for casting integrity, knowledge of defect formation, distribution and quantity is required. This is the challenge facing modellers. As these optimization software such as MAGMAfrontier [3] become more user friendly and the performance of computer hardware increases the requirement for accurate and quantitative defect assessment criteria will become even more acute.

Many liquid metals form an oxide film upon their free surface due to the reaction with the oxygen in the atmosphere. This extremely thin solid film, in the range of nm to µm in thickness, forms almost instantaneously and thickens with time. When the surface oxide film is entrained into the bulk fluid the film may be broken up by turbulence flow into numerous single entities known as oxide films. These oxide films act as a crack initiation sites upon solidification. These films do not bond within the metallic structure and are therefore weaknesses, which acts as an initiation sites for cracks to propagate from. The entrainment of oxide films into the bulk fluid has been shown to have detrimental effects on cast component integrity [4].

The direct modelling of the physics of the entrainment process is currently seen as unrealistic giving the processes complexity and current computational power. The modelling of a thin film in the order of µm in thickness on top of a volume of fluid yields significant modelling difficulties from the meshing perspective. If a single mesh capable of resolving the µm thick film was utilized the runtimes for a casting fluid flow simulation would be many orders of magnitude above what is reasonable. Even using an adaptive meshing technique, where by the mesh is dynamically modified during simulation, allowing a finer mesh to be implemented for the film and a coarser mesh for the bulk fluid, would be computationally expensive and outside of reasonable simulation times as the adaptive meshing procedure would be computationally very expensive.

Campbell's 2006 paper [5] summarised most of the methods researched for the modeling of defect entrainment in castings thus far developed. Recent work has both proposed new methods and further developed, and assessed, previously proposed methods of modeling defects. This has given further insight onto this important topic. A discussion of the currently available methods for assessing casting integrity both quantitatively and qualitatively are discussed below.

It appears that Campbell"s final, but possibly most important conclusion; "*the use of entrainment models to optimise filling systems designs for castings has huge commercial potential that has so far being neglected by modellers*" [5] has still not been adequately heard as there appears that significant research is required in to this topic, but few teams are presently active.

Many defect modeling topics relating to the casting process have been researched, including solidification and thermal modelling (porosity), die/mould based modelling (burn on, sand erosion, die soldering, die life prediction) and stress strain modelling (distortion, hot tearing). However, in this paper only the modeling of filling related defect assessment of the casting process is reviewed.

Although work on modeling porosity is not reviewed here (one such review of porosity modeling by Lee *et al.* can be found here [6]), it should be noted that published research has shown porosity to be linked to oxide film defects [7], [8], [9],[10]. This suggests that the accurate modeling of entrainment defects could potentially yield benefits in the accurate modeling of porosity.

It should be remembered that the accurate modeling of entrainment also has the potential to yield significant benefits in optimizing the manufacturing processes of chemicals, paints, food and cosmetics, where entrainment of surface films or gasses is often a process limiting parameter.

A variety of approaches into the methods of modeling of entrainment defects have been investigated. These can be largely split into two groups, the discrete and the indiscrete modeling of entrainment defects.

Indiscrete Modeling of Entrainment

Cumulative entrained free surface area

Work by both Lai *et al* [11] [12] and Sun *et al* [13] investigated using the difference in free surface area to describe the magnitude of entrainment. Little is known of the work by Sun *et al.* due to commercial sensitivities, although the authors reported positive results using the technique.

The work by Lai *et al.* [12] takes the instantaneous free surface area and plots it against time. This is then compared to the proposed instantaneous free surface area assuming the mould had been filled in a tranquil manner, to allow the excess of free surface area to be calculated. The work showed that the largest excess free surface area was during pouring from the furnace into the crucible and from the crucible into the mould. This highlights the fact that the quality of the metal entering the running system is of extreme importance to casting integrity.

This technique [12], although easily understood and requiring minimal computational power has one major drawback, namely; how to define the minimum free surface area should the mould fill quiescently. For very simple geometries comparison between differing geometries is possible, though time consuming. For complex geometries however, this could prove near impossible. Therefore, this technique is unsuitable to use for optimization except for instances where direct comparison can be made between two or more models (i.e. for models of identical geometry). This technique gives no distribution of defects but is felt to be nevertheless highly informative as it is a strong indicator of which stage of mould filling is likely to generate the most significant number of defects. The lack of ability to track the motion of the entrained defects also proved detrimental to the usefulness of this technique. To develop this technique an efficient algorithm to calculate the minimum free surface area is required.

Vorticity

Both MAGMAsoft [14] and Flow-3D [15] have developed techniques to identify and assess vortices within the bulk fluid during flow simulation of mould filling. This function is also available in CFD post processing software such as Field View, CEI and Tecplot. These analysis tools allow the vortex core location and axis and vortex magnitude to be defined. The problem arises however in filtering of the data. The bulk fluid flow in the casting scenario is usually in a highly turbulent regime, producing many vortices, filtering the data to only show those relevant to free surface entrainment can be highly problematic. The authors are currently unaware of any work which has been undertaken relating vortex assessment using a computational model to defect entrainment or casting integrity.

Cumulative Scalar Technique

A cumulative near surface scalar technique has been developed by a number of the commercial casting software manufacturers [16-18]. The technique works by assuming that oxide defects accumulate upon the fluids free surface at a constant rate; this oxide accumulation is described by a scalar parameter. This scalar once entrained into the bulk fluid at the free surface is allowed to gradually diffuse throughout the fluid and advect with the flow of the bulk fluid. This allows a final defect probability to be obtained. This is a simple and robust approach which neglects the physics involved in bi-film entrainment. However, the approach has been shown to yield results in accord with more sophisticated models and experimental data.

As stated by the Barkhudarov and Hirt [17], 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.

An almost identical technique is also utilised in smoothed particle hydrodynamics (SPH) [19-21]. SPH is a technique whereby the bulk fluid is divided into a series of discrete elements known as particles. These particles are then given properties and allowed to move within the constraints of a set of governing equations. SPH is a gridless technique where the particles can move anywhere within the domain and interact with each other following a set of defined physical rules. The cumulative scalar technique operates in the same way as that described previously but with the exception that the quantification is not constant, but defined by a relationship proposed by Backer *et al.* [22]. This is to try and quantify the mass of oxide entrained.

It must be remembered that these scalars diffuse within the liquid (Figure 1) unlike bi-film defects which remain as single entities unless torn. Therefore representing individual defects as a scalar quantity is always going to be problematic as the interactions between the defects, mould and liquid cannot be modelled.

MAGMAsoft Air Entrainment Model

An air entrainment model has been developed by MAGMAsoft as a mechanism to track small air bubbles transported by the bulk flow. The model is made of two main constituents; a venting model and an air entrapment model. The criteria MAGMAsoft use to define the quantity and threshold of air entrainment at the free surface into the bulk fluid is proprietary.

The venting model is the main mechanism for tracking air pockets; this tracks changes in topology of air pockets and calculates their thermodynamic parameters. Using this, the number of discrete air pockets and each pockets location is known, along with their density, volume, mass, temperature and pressure. Air pocket can collide with other air pockets and can merge or split. The venting (permanent moulds/dies) or permeability (consumable moulds) of the mould is modelled to allow accurate modeling of vented regions. The venting model can operate only on air pockets that are resolved by at least several mesh elements.

Air entrapment is a model that enables tracking air pockets that are too small to be tracked by the venting model. Air entrapment operates only on the air volume transporting it with the bulk melt velocity field. The model is valid for small bubbles. The air entrapment models give the user a contour map of air distribution within the melt volume.

Alongside their main air entrainment model MAGMAsoft have also implemented in their code, (although at the time of writing not all are available to customers) several scalar quantities aimed at helping the foundry engineer assess the likelihood of entrainment. These include flow length, material age, and wall contact time and are defined below:

- Flow length - Distance the metal has flown since entering the cavity
- Material age - Length of time the material has been in the cavity
- Wall contact time - Length of time the material has been in contact with the wall

Flow-3D Air Entrainment Model

Flow-3D have developed an algorithm to model the turbulent entrainment of air at a free surface [23]. The model works by assessing whether the turbulent energy at the free surface is enough to overcome the restraining effects of the surface tension and gravity. If the magnitude of surface turbulence is able to overcome these restraining effects then a series of equations are used to calculate a quantity of entrained air. This air is then entrained into the fluid and allowed to advect, dissipate and escape at the free surface. The bulking of the fluid with the volume of entrained air can be modelled.

The model has been validated on data collected by researchers in the hydraulic engineering fields. The volume of air entrained experimentally at hydraulic jumps, spill ways and plunging jets were used for validation of the model [23]. The accuracy of this data however, now has to be questioned due to recent research findings. The model does show an excellent correlation with the location of entrainment [23], even if the questions can be raised about the magnitude of the entrained gas, thus still making it an extremely valuable modeling tool.

Resent research in the hydraulic engineering field has shown that the scale of an experiment has an effect on the entrainment threshold (critical condition upon which entrainment commences), size and quantity of bubbles entrained. Traditionally, scaled down models of large civil engineering structures have been used to assess the flow and entrainment characteristics before construction commences. Recent work however, demonstrates quantitatively that dynamic similarity cannot be achieved with either the *Fr* or *We* numbers as has traditionally been assumed [24], [25], [26], [27], [28]. Results from Chanson show that small scale models, when compared to full scale, underestimate the energy dissipation and entrain fewer bubbles of a greater size for similar inflow conditions [26]. The entrainment threshold for a hydraulic jump has been shown experimentally to lie over the huge range of *Fr* numbers of 1 to 4 [29], [30], [28]. The effects of experimental conditions, *i.e.* inflow conditions and scale can now account for this broad range of results [31]. For a plunging jet entrainment has been shown to only occur when it is perturbed [32], [31]. Fluid jets with very high Reynolds numbers can impinge on a volume of fluid without initiating entrainment so long as their surface remains free of perturbations [33]. For a given jet velocity the volume of air entrained is proportional to the jet disturbance [31]. It should be noted that all the above research into dynamic similarity was undertaken using water and *not* liquid metals.

Dimensionless Number Criteria

The use of dimensionless numbers has been previously proposed for use in assessment of defect entrainment by Campbell [34] among others. Previous studies utilising the

Weber Number (*We*) (ratio of surface tension to inertial pressure) [35] and Froude Number (*Fr*) (ratio of gravitational pressure to inertial pressure) [35] include that of Cuesta *et al*. [36-37] and Isawa [38] respectively. The use of dimensionless numbers does not enable the tracking of defects. However, it does have the potential to allow the quantification of entrainment. It must be remembered that the greatest limitations for the use of dimensionless numbers for quantifying entrainment in casting systems is firstly their inability to differentiate between the many types of entrainment mechanisms, namely: plunging jets, fountains, bubble trails and colliding fluid fronts. Secondly, they are not able to assess entrainment in all regions, especially in a mould cavity of complex geometry, of the casting system.

Work by Isawa using the Froude number in the casting arena involved water modeling in a supposedly impermeable mould showed a *vena contracta* forming at the sprue to runner junction [38]. By calculating the dimensions of the volume of air present in this *vena contracta* and the *Fr* number of the incoming flow, an empirical relationship was then used to calculate the time a flow of that *Fr* number would take to remove the air in the *vena contracta*. The results matched closely with the experimental data. It is not clear whether this air was transported into the mould cavity by the hydraulic jump or escaped through the mould walls. The permeability of the mould to air is questionable, as the author states that after twenty-four hours of applying the surface coat, water hardly penetrated the mould walls. The permeability of the mould walls to air was not measured, and is therefore unknown. Isawa concludes that the higher the *Fr* number of the system, the shorter the time for the disappearance of the *'vena contracta'* and that this is desirable for an optimised running system. It would appear that the author is thus incorrectly recommending that the presence of a hydraulic jump, which is entraining both air and oxide film into the bulk fluid is advantageous.

Hernandez-Ortega *et al.* [39] used a combination of both the *Fr* and Reynolds (*Re*) numbers (ratio of viscous to inertial forces) to characterise the filling patterns of a vertical rectangular die using low and medium pressure die casting. This work, although not directly modeling defect entrainment, has shown both experimentally and using modelling that the *Fr* and *We* numbers can be used to characterise the flow form of water entering a vertical rectangular die. Four discrete flow forms were defined: transition, mound, palm and shell in order of increasing probability of entrainment occurring. This technique could be used to allow the foundry engineer to assess the likelihood of entrainment by calculating the *Fr* and *We* numbers of the flow entering a vertical rectangular die and see whether it is likely to be entraining. However further research is required to validate the technique for liquid metals and more complex die geometry.

Cuesta *et al.* investigated the influence of geometry n the critical velocity for free surface entrainment of aluminium. Using a commercial CFD software, and validating against previously published data, they modelled both round and rectangular cross section vertical in gates to assess the critical conditions at which free surface entrainment is initiated. The flow conditions through the in gate were assessed using the Weber number. This work suggested an entrainment threshold *We* number of 1.4 for the entrainment of oxide in liquid aluminium in square inlet channels, which is higher than the theoretical value of 1. The paper then goes on to propose the entrainment threshold lying in the range of *We* number of 0.5 - 1.5 for all channel shapes, geometries and materials. However, this work contains no experimental validation for these threshold values. The main findings of the work were that both the size and shape of the in-gate has an effect on the critical velocity at which entrainment will occur.

There are some questions over the work on the *We* number by Cuesta *et al.* which lead the authors to question its validity. Firstly the choice of a contact angle of 10° between the mould wall and liquid metal [36] seems unrealistic, it is widely acknowledged that a value of approximately 160° is appropriate for most liquid metals. Secondly, Cuesta *et al.* state that assessment of the conditions took place once the numerical modeling "proved to be accurate enough". However it is this author‟s opinion the models shown in the paper are in some cases inaccurate, Figure 2.

It seems that the use of dimensionless numbers for assessment of in-gate flows is an area of research which requires a more detailed investigation.

Reilly *et al.* [40], [41], [42] have used dimensionless numbers to create criterion functions with which to interrogate computational models for quantification of entrainment. The Froude number [35] (ratio of gravitational to inertial forces), Weber number [35] (ratio of surface tension to inertial forces) and Hsu number [43] (ratio of inertial to gravitational and surface tension forces) were used for the assessment of returning wave forms in horizontal runner bars.

A user customisation was programmed in *Flow-3D* to extract each of the dimensionless numbers at a determined frequency from the runner bar of the model [44]. To enable this to be achieved the flow regime was first characterised as one of four types as described in Figure 3. Once characterised the appropriate assessment technique allowed the extraction of the relevant velocities and length parameters to allow calculation of the dimensionless numbers within the runner bar. Upon completion of the model the instantaneous dimensionless number could be integrated with respect to time to calculate a single quantitative "total damage‟ value for each model. This allows the quantitative comparison of running systems.

This technique was validated against experimental work. Four moulds were cast containing tensile test specimens; two head heights (high and low), both with and without reticulated foam filters. The integrity of each system was assessed using the Weibull modulus [45]. The experimental procedure was modelled in *Flow-3D*, the models included the modeling of the pour. A mesh sensitivity study using a regular Cartesian mesh of 2, 4 and 6 mm side lengths was also under taken [40], [42].

The experimental data gave Weibull moduli of 38, 32 and 8 respectively for the high filter, low filter and low conditions [40], [42]. (the higher the Weibull modulus the greater the integrity [46], [4]). The high condition mould created tensile specimens with so great a degree of entrainment present (multiple visible bubble defects within the test specimen) that tensile testing was deemed as inappropriate. Scanning Electron Microscope (SEM) analysis was undertaken which showed the cause for specimen failure was consistent with those associated with entrainment defects, namely: oxide films, bubbles and micro-porosity [40], [42].

Examination and comparison of the experimental results and modelled results showed that they were consistent with one another, showing the same flow types. However due to being single phase flow it was not possible for the software to accurately model the large numbers of bubbles seen in some experimental conditions.

The *Fr* and *Hsu* numbers were seen to correlate with the experimental data, whereas the *We* number was not found to accurately predict casting quality. The *We* number showed a large difference in magnitude between the filtered and unfiltered conditions but incorrectly differentiated between the smaller order of magnitudes between the two filtered conditions and the two unfiltered condition.

The *Fr* data was tested for mesh sensitivity and was found to correlate with experimental data in the 2 and 4 mm mesh condition but not that of the 6 mm condition. The *Hsu* data correlated with experimental data in the 4 and 6 mm mesh condition but not that of the 2 mm condition. Analysis of the model suggested that this was indeed due to the sensitivity of the model to mesh size rather than a sensitivity of the *Fr* or *Hsu* criterion, i.e. the modelled flow was different in the different mesh sizes. This sensitivity to mesh size does however severely limit the use of dimensionless numbers for optimization purposes at this stage of development.

The ratio of inertial to gravitational forces (*Fr* number) appears to provide the best representation of entrainment within the runner bar. The high energy flows usually present within a runner bar often overcome the surface tension forces. An example of fluid energy overcoming surface tension forces can be seen in flow structures including: plunging jets, returning waves and rising jets. If the surface tension forces were sufficiently great then there would be no entrainment even for the free surface profile of a return wave as the surface tension would restrain the free surface preventing the entrainment of air packets. Therefore, the ratio of inertial to surface tension forces (*We* number) does not well represent the likelihood of entrainment in this scenario. It should be remembered that the surface tension of water is approximately 10% that of liquid aluminium.

Whilst these results appear encouraging, the technique requires further developments; these include the quantification of the entrainment threshold in liquid metal as opposed to water, and establishment of a relationship between the dimensionless numbers and degree of oxide entrainment. The effect of the changing surface tension with age of the oxide file could also make defining the entrainment threshold problematic as it is likely to be extremely sensitive to surface tension. The definition of these entrainment thresholds may be possible by further developing the work of Pita *et al.* [47]. This work has simulated the movement and breakup of a thin solid film in a volume of fluid and as is discussed later in this review article. In this investigation the theoretical entrainment threshold of 1 and the oxide entrainment rate being linearly proportional to the dimensionless number was used. Work by Ohl *et al*. [33] and Chanson *et al.* [26], [48], [27], [28], has shown that the magnitude of undulations upon the fluids surface and the physical scale of the entraining phenomena greatly impact the magnitude of entrainment. This makes it difficult therefore to quantify the magnitude of entrainment without assessing these factors alongside the dimensionless number. However their minimal computational overhead makes this technique attractive to industrial and optimization applications should they gain further development to resolve these issues.

Multi-phase modeling

Bubble trails have been shown to be highly detrimental to casting integrity. The accurate modeling of bubbles; their entrainment, advection and coalescence is an important element of the modeling of casting entrainment. By modeling both the bulk fluid and surrounding gas (two phase modeling) it has been possible to describe the entrapment, advection and coalescence of bubbles within the melt [49], [50]. However further development is still required before these codes are viable as commercial software packages. Initial results show correlation of bubble motion, coalescence and separation with experimental data. These software are, as expected, computationally highly intensive when compared to single phase flow modeling due to the substantial additional complexities of modeling the second phase. However, modeling both the liquid and gas phase appears to be the only way to correctly model highly aerated flows.

It appears that currently the developers of two-phase-focused software are concentrating on developing the flow modeling rather than the addition of models for the quantitative modeling of casting defects. At the current time the authors are unaware of any two-phase-focused software incorporating quantitative defect prediction models. However, this does not mean that they have not been successfully validated [51] and applied qualitatively in the application of defect prediction and process optimization [52].

The use of any two-phase flow software to quantify or track the defects produced by the entrained gas has yet to be under taken, although the addition of one or more of the techniques described to model discrete defects within this paper has the potential to yield good results.

Modeling of Discrete Defects

Methods have been developed to model the entrainment and advection of discrete defects. This is obviously very challenging and usually requires greater computational expense than the indiscrete methods described previously. However there are some considerable advantages associated with this approach, namely: entrainment mechanisms can often be identified and the final defect location can be obtained.

There are however some current issues which require further investigation. Many of the techniques described below have had to make assumptions about: both physical characteristics of the defects and their behaviour, critical entrainment thresholds and interaction of defects with both mould materials and each other. It is often not the practical modeling, but determining exactly what mechanism or physical situation to model is the greatest challenge facing modellers. For this reason, modellers will have to work closely with experimentalists for effective progress to be made within this field.

The models for predicting porosity to use in heterogeneous nucleation have thus far concentrated on bubbles as sites for porosity formation. Further development of discrete film entrainment techniques would investigate the possibility of modeling oxide film defects as sites for porosity nucleation.

Many of the following techniques used to model discrete oxide film entrainment utilise particles to represent entrained defects. This comes with some currently inherent issues, often caused by not having understanding of the physical behaviours of oxide films in the real world. Further research is required into the following topics, namely:

> Many of the particle models within the software have had no experimental validation. It is only current work by Griffith *et al.* [53], [54] which will allow the possibility of accurately assessing a simulation software particle tracking model. The particle-fluid coupling has only been assessed qualitatively thus far [55].
>
> The properties of oxide adhesion to mould walls is not fully understood. Obviously, the adherence of oxides to mould walls can greatly affect the models results. Carlson *et al.* undertook investigation [56] into the adherence of re-oxidisation inclusions onto mould walls in steel. Based upon these qualitative findings they allowed re-oxidisation inclusions to adhere to the mould walls in their model. However, it is felt that the mould surface, mould material, velocity (both magnitude and direction) and defect properties will all affect the defects adherence to the mould wall. The coefficient of restitution used in the models determines whether particles adhere to mould walls or rebound with an energy

loss. There has been no conclusive research into the adhesion of oxide films to mould walls; therefore, this assumption has no experimental validation. This can obviously have a huge effect on the final location of defects.

Although many discrete particle entrainment techniques do define and track entraining events they currently do 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. Therefore, it is not possible to categorically state that the number of particles entrained correlates with the area of quantity of oxide film entrained and thus damage to the material. However, the greater the numbers of defects present, the greater the probability of a highly damaging defect which initiates failure being present. It is anticipated that future development of the code could define the particle size as a function of the area of entrained oxide film.

Oxide films are individually unique, varying in size, shape and density. However, many models are not capable of modeling this. The particles are commonly specified as spheres of either constant density and varying size, or varying density and constant size. 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 and the generic properties to represent individually unique oxide films is currently not able to be validated due to the lack of experimental data.

Agglomeration of entrainment defects is a difficult subject as 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 [34] and large dross defects [56] 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.* [56] (dealing with re-oxidation rather than oxide film inclusions) allowed particles to agglomerate as a way of easing the computational load and to more accurately describe the characteristics of oxidisation inclusions in steel.

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 [57], although this work is not conclusive. Currently this is not accounted for the below models.

The changing the film‟s morphology (for example a large thin film becoming screwed up‟, folded or creased) between its formation and its final form in the solidified material is not accounted for. The morphology of the particle will have an effect on its motion due to a change in drag forces; this affect is unaccounted for in the current models.

Bubble Entrainment

A major omission from many casting software is the ability to model correctly the entrainment of air into the bulk fluid during casting. Defects caused by the entrainment of air into the bulk fluid include bubble trails, splash defects and entrapped bubbles. Bubble trails are hollow cracks (tubes) which create leak paths through the casting [58], [59], [60]. Entrapped bubbles (bubbles which do not escape from the bulk fluid) are commonly incorrectly assumed to be created through the rejection of gas upon solidification. If the bubble is near the surface it is assumed that it is the result of some reaction with the mould or mould coating. Should a bubble breech the free surface of the fluid during the filling of the cavity, small droplets may be produced which either adhere to the mould walls or re-enter the melt, these are known as splash defects. These fluid droplets have an oxide skin around them preventing recalescence with the melt.

The direct simulation of the bubble entrapment and subsequent effects of the bubble have been avoided. Full physical modeling of bubble entrainment would require the modeling of bubble entrapment, its advection including the drag forces placed on the bubbles motion by its oxide trail the bubble trail and bubble agglomeration. However the lack of knowledge of the film strength obviously complicated matters. Most available commercial packages could describe the initial entrapment of gas or void regions caused by macroscopic fluid flow scenarios, such as the "rising jet or fountain effect", where a volume of air is encapsulated by the fluid. However, most of the currently available casting software only consider the bulk fluid to be present in the model (single phase modeling). A bubble can only be modelled if the bubble size is greater than the size of a mesh cell. This obviously has a huge effect on the minimum bubble size it is possible to model before simulation time becomes unjustifiable due to the increase in computational time caused by the use of a fine mesh.

Although many commercial software codes have the ability to model bubbles with pseudo two-phase flow as discussed by above, currently commercially available software capable of modeling the two-phase flow (which is required to model large scale bubble entrainment and detrainment effectively) for complex casting shapes often struggle to meet the runtimes many industrial users demand.

The use of pseudo two-phase flow for permeable moulds can be highly problematic. The entrapped air volumes can be specified as adiabatic and are initially trapped at atmospheric pressure. For the case of sand moulds where it can be assumed that the mould is permeable to gas within the mould cavity, the use of this method proves difficult as it is not possible to specify a mould material permeable to the entrained gas and atmospheric gas within the mould cavity. Instead vents have to be added, however it is unreasonable to add vents to every mould cell. Therefore, gas pockets which are either entrapped against the mould walls or entrained within the fluid cannot be vented through mould walls and are therefore often incorrectly trapped within the mould volume (unless a pre-placed vent is present within the entrapped volume). This can cause the flow fields to be incorrectly modelled and sometimes gives pressure convergence issues. Obviously using the bubble model is not unrealistic for impermeable dies where vents can be added in the same location as the real vents in the die. The modelling of mould venting of consumable moulds such as sand and investment moulds is a topic that would benefit from further research and development.

As yet the modeling of the bubble trail with all its intricacies has yet to be attempted. This is most likely due to the perceived difficulty of even obtaining experimental data on the physical properties of the bubble trail and creating a bubble trail model which has practical use. It is highly likely that if bubble trails were to be modelled the extreme computational expense would be too great to allow its introduction into commercial software or to run casting models of even moderately complex geometries and scale. Therefore, it is felt likely that other models approximating the bubble trail may be the solution to this problem.

Single phase modeling software such as that used in the foundry industry are limited to the size of mesh they can use due to the requirements for fast results [61]. These single phase software require, at minimum a single cell devoid of fluid to be able to define a bubble. Therefore to track small bubbles such as those entrained by a returning back wave, an extremely fine mesh is required. This produces runtimes many magnitudes longer than is acceptable in most industrial scenarios. Work by Ohnaka *et al*. has used particles to represent and track entrained bubbles for the prediction of porosity [62], [63], [64], [65]. This technique has been developed to remove the need to use extremely small mesh element sizes to track small bubbles.

To allow the tracking of these small bubbles Ohnaka *et al.* developed a technique to place particles when the void region becomes too small to be defined by the mesh. These particles are then tracked and their final locations defined. These are then used to define the location of heterogeneous nucleation sites for of gas porosity [62], [63], [64], *[65].* This technique is an adaptation of that developed previously by Tomiyama *et al.* [66]. This allows the tracking of the bubbles without the computational expense of small mesh cell sizes. They found the technique gave results which correlated well with experimental results. However the technique was found to be extremely sensitive to the particles buoyancy force (this is related to the particle density and size).

Modeling of Oxides in Steels

A method based upon the formation of oxides from nuclei was used as a methodology to model defects in steels. A team from Iowa University lead by Beckermann [67], [68] introduced particles into the melt and allowed them to grow when upon the free surface. The particles were either added to the incoming fluid stream, or placed upon the free surface so as to give a minimum free surface particle density, i.e the number minimum number of particles upon a free surface is defined by the user and code add particles if required to achieve this value. When the particles are sub-surface, only their advection is modelled, their growth is not permitted. The particle motion is tracked until solidification and agglomeration of colliding particles (oxides) is permitted. The final location of these particles and their size give probabilistic representation of the likelihood of entrainment defects being present.

Carlson and Beckermann have further developed and undertaken validation work of this steel inclusion modeling technique showing good correlation with a number of experimental validations and has been successfully used in industrial applications [56]. They have created a very elegant and seemingly robust method of modeling oxide inclusions in steels, and shown it to give reliable results in industrial applications.

Modeling the Folding Mechanism

This method, used by Lin *et al* and Dai *et al* [69], [70], [71], [72] models the entrainment of bi-films through the folding of the free surface. It is therefore only able to model certain entraining phenomena such as returning waves and folding surfaces.

The methodology used by both Lin and Dai is based upon placing particles on a fluid‟s free surface to represent the oxide film. Particles are added if the surface is expanding, and when a particle is added to the model then all particles are re-labelled. The particles also have to be replaced onto the fluid‟s surface at every time step, should the free surface form have changed. This suggests that the technique may be computationally intensive. These techniques have also only currently been applied in two dimensions, currently expansion into three dimensions would severely complicate the programming required and further increase the computational effort.

Lin assumes the oxide films to be present between neighbouring particles and calculates the strain the film is under by tracking the movement of neighbouring particles. Should the strain exceed the strength of the film, further particles are added as the film is assumed to have torn and immediately new oxide film has been formed. The model is able to assess the entrainment of air bubbles into the bulk liquid by surface turbulence. Once a film is entrained in the bulk material the tracking points are no longer adjusted to fit the free surface and it is assumed that there is no atmosphere for oxidisation within the bulk material. Therefore no new particles are added should the film break due to excessive stress. The location and number of these entrained films are tracked.

Dai‟s approach varies slightly by assessing the surface normals of the films. Should they be pointing towards each other and their velocity vectors obey a predetermined mathematical rule (meaning that the films would converge) then entrainment is deemed to occur. This model was then compared to experimental data and deemed to be qualitatively consistent.

One major drawback with this model is that it is currently only implemented on the OFET 2D CFD (computational fluid dynamics) in house code. The authors are unaware of any shape casting simulations undertaken with this software, presumably due to its current 2D limitation.

The authors would like to make three comments on the work undertaken by Dai. Firstly the code was validated by mechanical testing of samples cut from cast plates. It should be noted that the samples were initially tested by subjecting them to a four-point bend test. The broken samples were then subjected to a three point bend test [71]. Obviously the results of the latter three point bend test have to be regarded with some caution, as the effect of the initial test on the strength of the sample is not quantifiable. It is likely that this initial test opened up crack initiation sites, potentially severely weakening the samples.

Secondly it should be noted that the comparison of the down-sprues on both the vortex and rectangular runner validation moulds are different [71]. The sprue inlets and pour basins are identical on both, however the sprue exit is 75 mm^2 on the rectangular runner and 150 mm^2 on the vortex runner. Using Campbell‟s design rules the maximum sprue exit area for a 175 mm tall sprue is 105 mm^2 [34]. It can therefore be seen that the rectangular runner has a choking sprue whilst the vortex runner‟s sprue is oversized. This will mean that there is effectively a plunging jet occurring as the bottom of the down-sprue until there is enough head height from within the casting cavity to back fill the bottom of the down-sprue. Dai‟s work suggests that the oxide entrainment was by the folding of films within the casting volume, as was modelled. There is a large probability however, that there were a significant number of young oxide films introduced to the plate castings which were entrained in the down-sprue of the vortex runner casting. This has not been accounted for in the model.

Thirdly, upon inspection of the models run using the OFET code the flow can be seen to be perfectly symmetrical (Figure 4). It is known from real time x-ray results that this is unrealistic, Figure 5 [73]. The reason for this flow behaviour is assumed that a pressure boundary was applied to the bottom of the plate as an inlet condition as the 2D OFET code was unable to model the running system. The validity of comparing the incorrect computational models to the experimental data is therefore questionable.

It should however be stressed that this method of modeling the entrainment of oxide films through folding of the free surface does have merits, namely: quantifiable output (number of particles in the model/ critical volume can be counted) the motion of the defects can be modelled. However the authors feel that further investigations and development are required to exploit its full potential.

Modeling of Oxide Entrainment

The work by Ohnaka *et al*. on modeling bubbles in single phase flow [64]was then further extended to include the modeling of oxide entrainment in aluminium castings [74]. Making the assumption that the aluminium surface which is exposed to the atmosphere instantly forms an oxide film, the free surfaces are then assessed using defined physical rules [75] to see if they collide, thus entraining oxide films. If entrainment occurs, marker particles are placed to represent the entrained films. Their advection within the flow is then calculated to define their final locations upon solidification.

The number of entrained oxides per unit area is estimated as a function of collision velocity and alloy composition the parameters of which were defined through unpublished experimental work. The average surface area of the broken oxides is estimated using a function of the collision surface area, the surface area of a broken oxide and the number of entrapped oxides. The function means that at larger collision velocities, more but smaller oxide films are entrained [74].

The judgment of a free surface collision is classified by assessment of the velocity vectors, distances between particles and the time period. This methodology allows the entrainment caused by fluid jets, bubbles, colliding fronts, impinging flows and return waves to be modelled. Further validation with respect to the modeling of oxide defects rather than that of porosity which has been so far undertaken [74] would give a greater insight into this methods validity for the modeling of oxide film defects.

Oxide Film Entrainment Model (OFEM)

Research by Reilly *et al.* used a very similar methodology to that developed by Ohnaka *et al.* [54], however the implementation varied due to factors associated with the software. In this work an oxide film entrainment model was developed as a *Flow-3D* customisation [76], [77]. The model assesses the velocity vectors, fraction of fluid at both the beginning and end of a time step, orientation of the free surface normal and surface area of free surface cells and defines entraining events by the use of Boolean logic criteria. Once an entraining event has been detected a particle of determined size and density is placed to represent the defect. The particles motion is then modelled.

Upon solidification the particles within defined critical volume(s) or the whole casting can be counted to allow quantitative analysis of the casting system.

The experimental work of Green and Campbell [4] was modelled in *Flow-3D* and the OFEM applied [76], [77]. This work consisted of pouring moulds, both with and without a 10 ppi reticulated foam filter at the bottom of the down-sprue. The test specimens were then tensile tested. The results showed the filtered condition to give test bars of greater integrity than that of the unfiltered condition; Weibull modulus [45] of 37.7 and 19.7 respectively. The average number of particles in the gauge length of the test specimens was compared to that of the Weibull modulus.

The modelled results agreed with those found experimentally. 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). 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 conclusive validation of the technique.

The experimental results show the defects “easily identified as oxides”[4] 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 incorporation and transport of particles within the liquid metal as reported in this work is not unique. Algorithms for doing so having been described previously by Yang *et al.* [78], [71] and Ohnaka *et al.* [64]. However, it is considered that this work is an initial evaluation and quantitative validation of a promising technique for modelling entrainment defects in shape casting. This is also a code targeted at optimization, and thus incorporates quantitative assessment techniques of the final particle locations.

Modeling of Oxide Film Deformation

Work by Pita *et al.* [47] has modelled the transport and deformation of a single oxide film within a fluid volume. Although this technique is currently not aimed at defect entrainment prediction it is included as it has the possibility to be developed into a key constituent in the development of accurate defect entrainment models. It is therefore included here as it is felt to be of the upmost importance.

The technique has in two dimensions shown that it is possible to accurately model the advection and large scale deformation of a solid film within a fluid, and the effect this solid deformation has upon the fluid motion: *i.e.*coupling of a fluid and deformable thin film.

Pita *et al.* state that they aim to further develop this technique by simulating a more realistic model and including a breakage criterion for the film, and solidification elements (phase change and solute transport) [47]. The addition of the ability to model a breaking film will allow the direct modelling of film entrainment for simple models.

With the present state of computational hardware it seems unlikely that this technique can be applied to large scale castings in the near future due to the computational intensity of modeling numerous films (which require the micro flow to be simulated) alongside the macro flow and solidification. However, the technique may play an important role in gaining insight into the physical behaviour of oxide films, of which surprisingly little is definitively known.

The work shows promise for the applications in modeling the unfurling of oxide films in castings, which is believed to be one of the mechanisms of porosity formation [34]. Thus far no evidence has been published to categorically prove or disprove Campbell"s theory. If this technique can be developed into a three dimensional model then the possibility of modelling this phenomena will become a reality.

A significant step in the development of this technique would be the introduction of a free surface within the model domain. If the film can be made to deform upon the free surface and break then the possibility of modeling directly the breakup and entrainment of the film will become a reality. Although it has to be expected that this would be extremely computationally intensive, thus ruling out the possibility of full scale casting simulation it would allow the determination of entrainment thresholds. The accuracy of many current entrainment models is severely reduced as the entrainment thresholds are not known. If simple models can be simulated to allow the definition of entrainment thresholds for different entrainment phenomena, with assessed parameters including: material properties, oxide age (thickness), fluid velocities and free surface topology then the accuracy of many current entrainment modeling methods could be greatly improved. The addition of these entrainment thresholds would solve one of the major questions in entrainment modelling; under what conditions does entrainment commence?

The second significant difficulty, associated only with the discrete modelling of defects is the correct modelling of advection and adherence properties. On this front the current model by Pita *et. al* is a significant step to being able to assess the accuracy of the current methodology of using spherical particles to represent entrained films which is used by many of the discrete modelling techniques. Although once again challenging to validate, a three dimensional model containing two or more films would allow the assessment of the representation of thin films with spherical particles and the interaction between two films when they collide. The ability to assess the deformation of the film during advection within a flow and assess its velocity within a known flow field, will aid the assessment of whether thin films tens to hundreds of μm in length and only μm in thickness within a fluid can be modelled as a continuum, or whether they have to be modelled individually with a drag coefficient which requires determining and may be time dependent if the films morphology changes with time. The re-oxidisation inclusion model [67], [68] currently allow the agglomeration of particles based upon qualitative evidence, this also eases the computational load by reducing the number of particles present within the model.

The ability to model a breaking film would potentially allow the assessment of film dimensions for given flow parameters for a given entrainment phenomena. The use of this data could be highly beneficial in improving the accuracy of discrete modelling techniques.

The ability to mode 3D films would allow the modelling of bubble trails. These tube like structures have thus far never been modelled but are widely believed to be highly detrimental to casting integrity [58-60]. The ability to model these tubes would allow insight into under what conditions the bubble trails are torn so as to try and understand not only their formation but their behaviour under common casting conditions.

Although the development of the technique of modeling the deformation of an oxide film has the possibility to be extremely powerful, it must be considered that validation of these techniques will be extremely challenging. Oxide films are small, tens to hundreds of µm in length and only µm in thickness, and invisible to the naked eye and still challenging to identify even with more sophisticated techniques such as using a scanning electron microscope. It is suspected that a representative experiment rather than an experiment using liquid metal or indirect qualitative evidence will be all that can be achieved in respect to validation models using these techniques.

Summary

The modeling and quantification of defect entrainment in the casting scenario is in its infancy and is an extremely difficult proposition due to a number of complex problems which have to be addressed. One of the most difficult of these is not the actual modeling of the defect but instead acquiring the knowledge of what to model. For example: do oxide films agglomerate if they collide, do oxide films stick to the mould surfaces and or under what conditions, what are the characteristics of oxide films created through different entrainment mechanisms and how do oxide characteristics affect the motion of defects within the melt? These problems require experimentalists to work alongside modellers to make further progress in the modeling of entrainment defects in castings.

However there are currently a range of techniques available to the modeller, as summarised in Table 1, which providing their limitations are recognised may shed light on the quantity, entrainment location and or final location of casting defects.

Conclusions

In this article the published methods of modeling entrainment defects in metal castings have been reviewed and the topics requiring further research have been highlighted. The topic of modeling entrainment defects in casting has received little attention in recent times despite its obvious commercial significance. The simulation of many phenomena has not yet being undertaken due to the complexity and lack of physical understanding.

However, the modeling of defects has been shown to be achievable and advantageous. One such example is the modeling of oxides in steels has been elegantly undertaken and validated by Carlson *et al [56, 67-68].* It is hard to see where to further develop this model without new experimental evidence to giving further insight into the properties, life cycles and behaviours of defects in steels.

The development of quantitative defect modeling techniques is difficult and complex, but of great industrial significance, and therefore further research is urgently required.

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Figures Captions

The Present State Of Modelling Entrainment Defects In The Casting Process

Reilly et al.

Figure 1 - Flow 3D Defect Tracking Scalar example. Diffusion of oxide scalar can clearly be seen (Barkhudarov and Hirt, 1998).

Figure 2 - Modelling versus experimental results from Cuesta *et al*. Experimental results are outlined in white, modelled results shaded in grey (Cuesta et al., 2006a, b). a) has a *We* number of 4.7 and b) 2.3

Figure 3 - Flow Type schematics for dimensionless number models. Where *v* is the velocity and *l* is a length (Reilly 2010).

Figure 4 - Example of OFET 2D oxide tracking model used for validation of the technique (Dai.X 2005).

Figure 5 - Real time x-ray example of flow in a cast plate (1995 benchmark test, 1.75 s) (Sirrell *et al.* 1995). This is the experimental data which was modeled by Dia *et. al* (as seen in Figure 4).

Table 1 - A summary of the benefits and limitations of the major defect modelling techniques which have been explored.

Figure 1

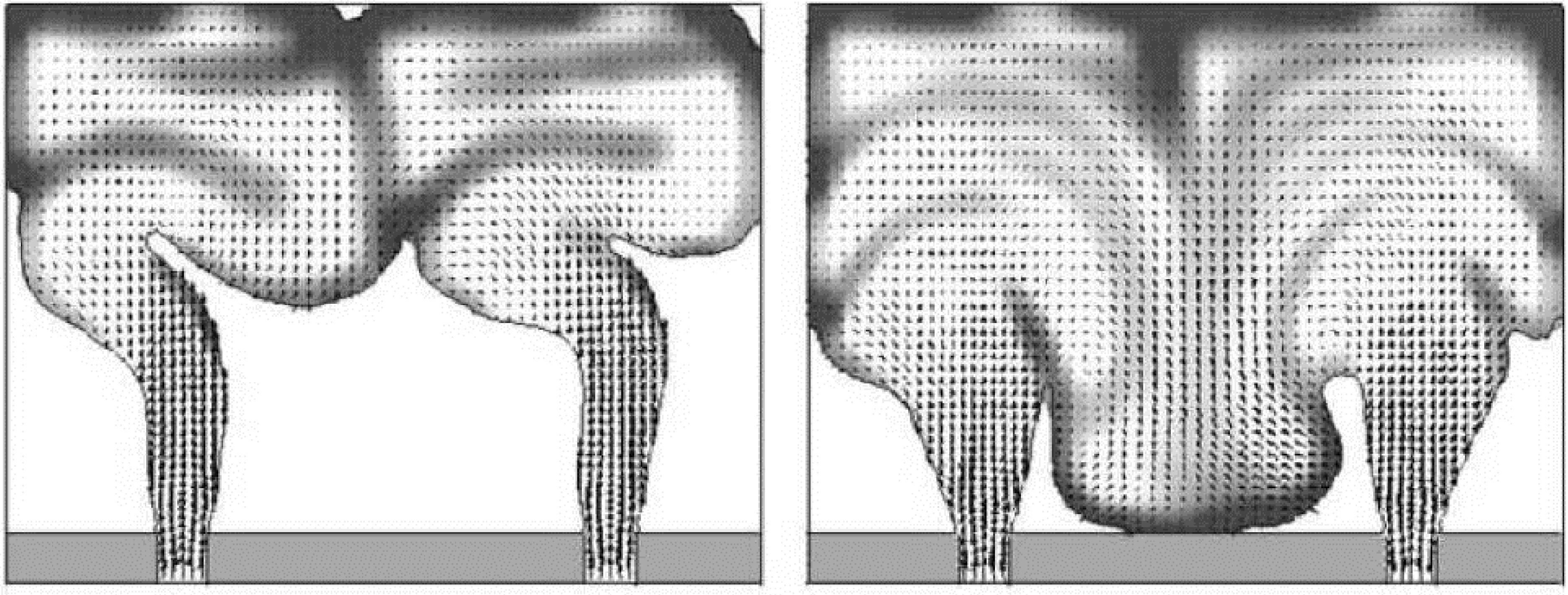


Figure 2

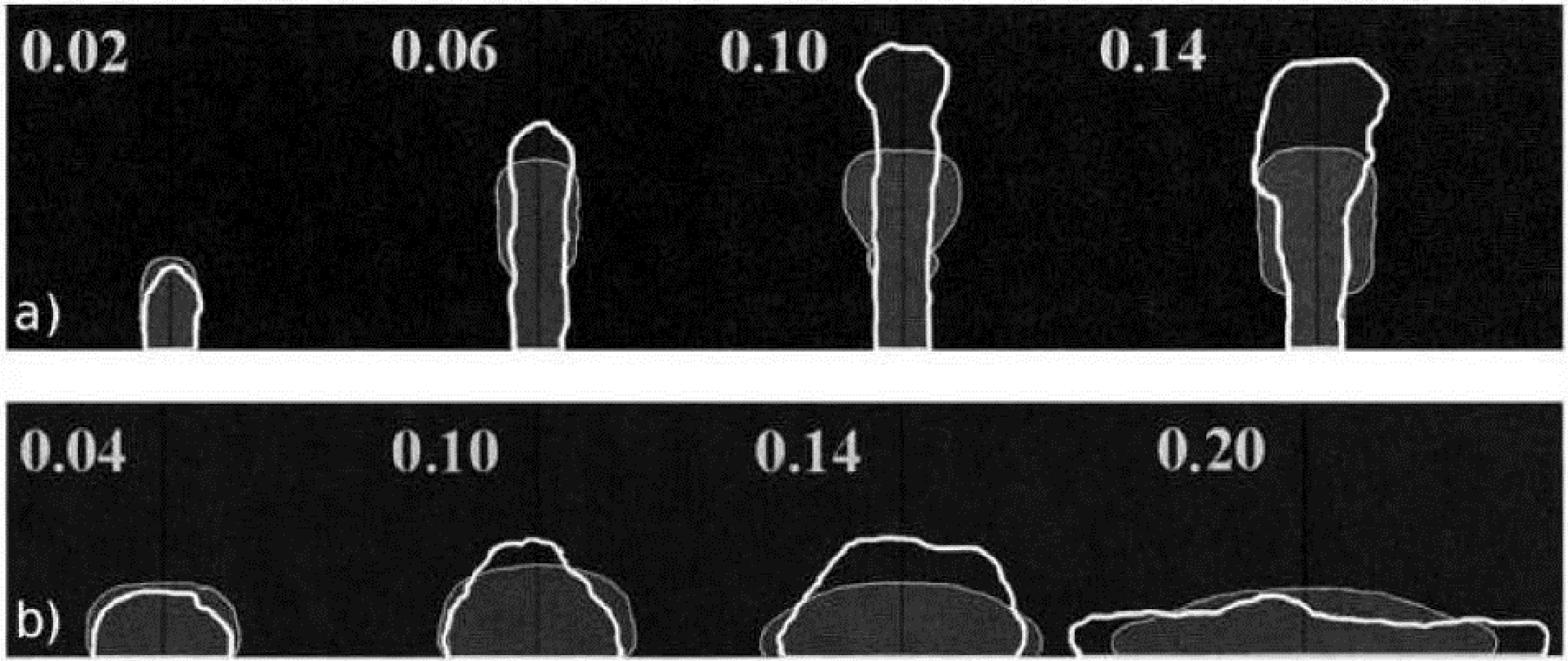
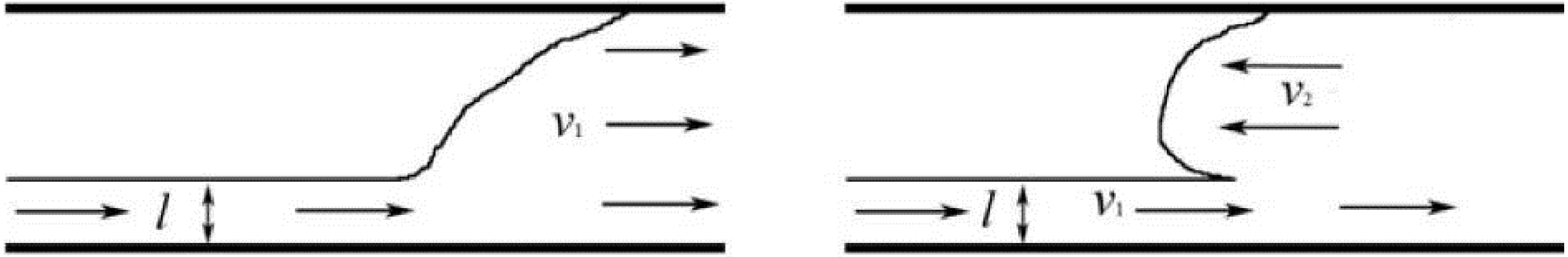
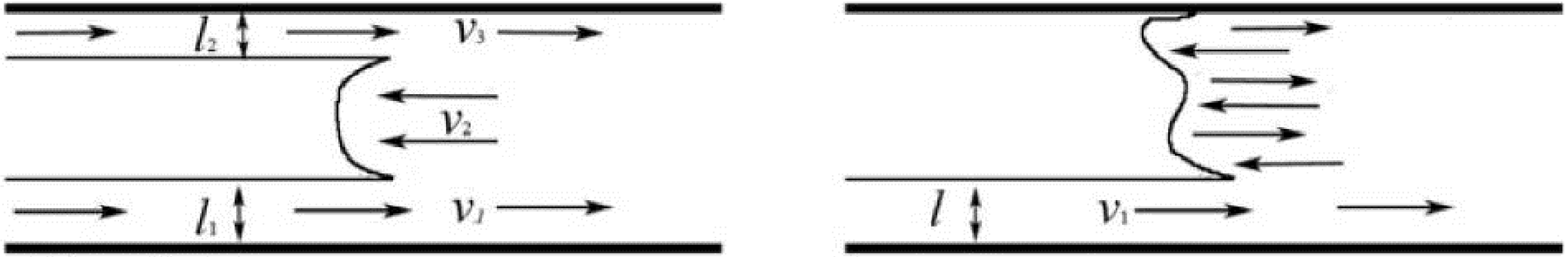


Figure 3



a) Flow Type 1

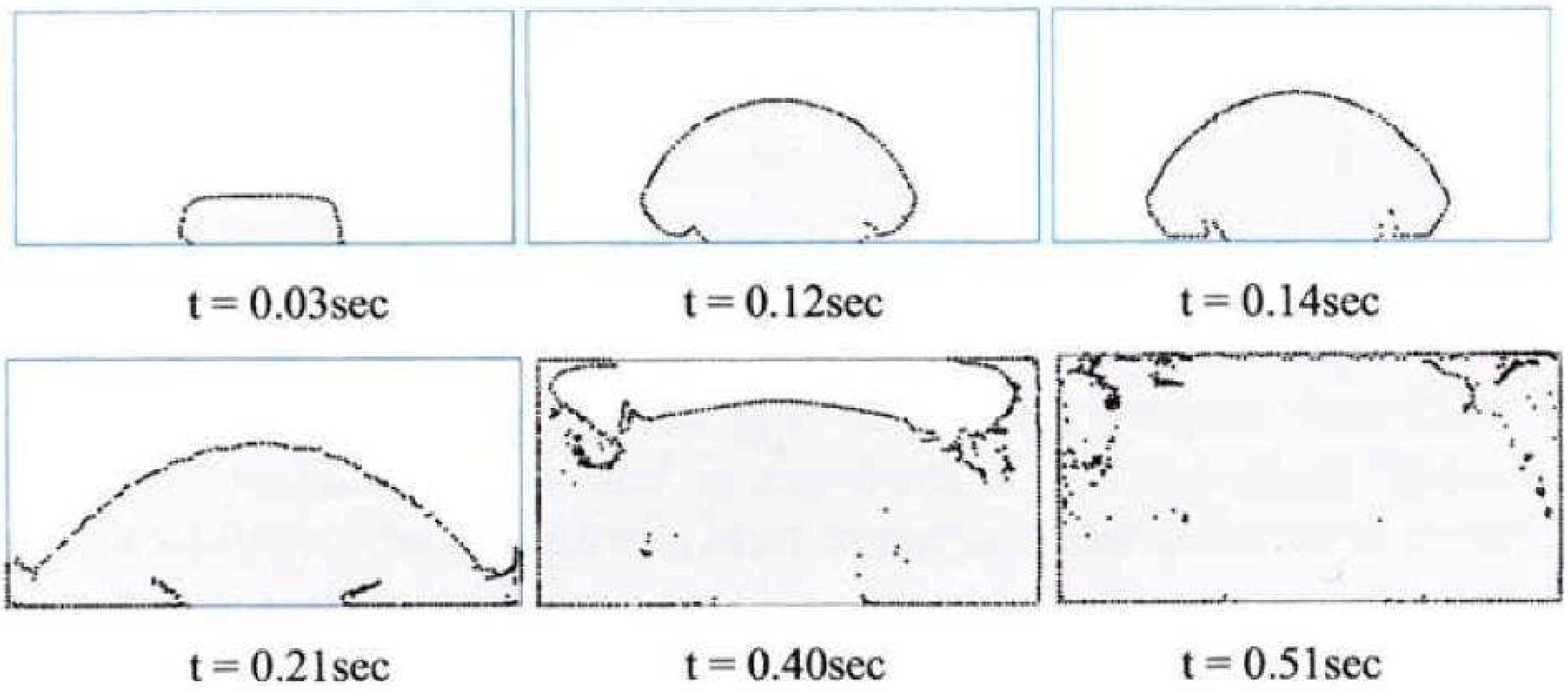
b) Flow Type 2



c) Flow Type 3

d) Flow Type 4

Figure 4



t = 0.03sec

t = 0.12sec

t = 0.14sec

t = 0.21sec

t = 0.40sec

t = 0.51sec

Figure 5