

**Numerical modelling of shrinkage defects induced by the feeding
flow in aluminium castings**

**Numerieke modellering van krimpdefecten geïnduceerd door de
toevoerstroom in aluminium gietstukken**

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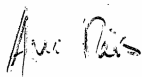
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Summary

This thesis presents a newly developed 3-D model that is capable of explicitly predicting the formation of shrinkage defects in castings, as a function of interacting continuum phenomena, free surface flow, heat transfer and solidification, in complex three-dimensional geometries. The developed physics-based model for shrinkage defects intends to capture the difference in solidification behaviour of skin freezing material and mushy freezing alloy by predicting location and extent of internal and external shrinkage.

In the present model it is assumed that the volume deficit due to shrinkage can only be compensated by the two following phenomena: depression of the outside surface or creation of internal porosity, which can be started on the surface or in the interior of the casting. As long as the metal is still liquid after pouring, the shrinkage of the material is compensated by feeding from the top of the casting, driven by gravity. At some instant, a solid layer will grow inwards from the mould interface, enclosing a liquid region. To compensate the mass deficit within the liquid region, a flow of molten metal has to be generated through the solidifying layer. This flow occurs through the emerging dendrites and will present an increasing friction, resulting in a pressure drop across the solidifying layer, which can cause a variety of problems.

The proposed model considers that liquid may be sucked from the surface area, which is particularly likely in long-freezing-range alloys, and consequently the external surfaces of the casting may sink to accommodate the internal shrinkage, or from obtuse angles in shorter-freezing range alloys, resulting in internal porosity initiated from the outside and connected to it. In short freezing material, due to the skin solidification, these mechanisms can be disabled in an early stage. If none of the mentioned mechanisms is activated, internal porosity may be nucleated.

In this model, an element that meets any of the preceding conditions becomes a free surface element. A free surface element is an element where no conservation law is applied and therefore melt can flow from the element to feed the casting. If the element has a neighbour element that is not containing metal, then this element is considered a free external surface, and a surface sink or a surface connected porosity will be generated. On the other hand, if the element is surrounded by elements containing metal an internal free surface is created, initiating an internal porosity.

A continuum formulation is used to describe the transport of mass, energy and momentum. It is assumed that during solidification the driving force for flow is shrinkage. A Darcy type source term has been included in the momentum equation to account for flow resistance in the mushy zone. A Volume of Fluid (VOF) free surface model is used to describe shrinkage defects, i.e. external surface depressions and internal shrinkage porosities, while ensuring mass conservation in the casting. By coupling the feed flow, pressure and solidification calculation for predicting shrinkage defects, a complete methodology that enables the possibility to show dynamic shrinkage geometry in the casting and feeding system is presented.

The computational approach exploits a compatible set of finite volume procedures extended to unstructured meshes. The implementation of the model is described together with its testing and validation.

To illustrate the features of the developed model, a simple geometry is used to perform a number of theoretical simulations that exhibit well known features of shrinkage related defects. To put in evidence the different morphology of these defects the behaviour between two alloys with a binary eutectic constituent, a short freezing (small interval between T_{liq} and T_{sol}) and a long freezing alloy (large interval between T_{liq} and T_{sol}), were analysed and compared.

The results showed internal and outside shrinkage defects depending on the freezing range of the metal. The result showed that short freezing alloys are more prone to internal shrinkage

porosities than long freezing alloys where shrinkage is noticeable in the form of surface sinks.

In order to evaluate the influence of the considered model parameters, a simple test case named “cup test” was experimentally obtained and a corresponding numerical simulation performed. The objective of this testing was: to identify a parametric range for the coefficient of permeability (K_0); to establish a porosity critical pressure/criteria, P_{crit} , that could be used in complex shape casting simulations; to analyse the influence of solidification interval and mesh sensitivity.

Two typical aluminium alloys used in casting, AlSi7 and AlSi12, were selected. The first alloy, AlSi7, can be considered a long freezing aluminium alloy. The AlSi12 is considered a short freezing alloy (almost eutectic composition). From numerical results it was clear that permeability had a significant influence on the macroporosity/voidage formation as might be expected. For a high permeability, the metal can flow to feed the solidifying areas sufficiently well to avoid the deep in upper level, or as in long freezing alloys to avoid the sinking of the walls. However, for low permeability, the feeding flow from upper level is severely restricted resulting in a more profound sink in the top for the AlSi12, and in AlSi7 this is revealed in sinking of the wall. The impact of initiation pressure was very small. Once the initiation pressure reaches a certain level, the simulation results are insensitive to this parameter. Experimental parts were obtained. The shapes revealed several forms of shrinkage defects. The different top geometry obtained in each alloy was observed. In the case of AlSi12 the top surface presents a deep sink, whereas the AlSi7 has a much flatter surface. Also, some internal porosity is visible in both alloys. In the AlSi7 this porosity is smaller and more uniformly distributed.

The experimental and numerical results are compared in order to find the best fitting situation. The appropriate parameter range which adequately reflected the main experimental observations became quickly discernible.

Another test case, “3-D complex shape”, was designed and performed numerically and experimentally. When designing this geometry the idea was to reproduce a real casting condition, part and feeding system, while maintaining the geometry as simple as possible to

better identify the variables directly enrolled in shrinkage feeding. Another requirement was to obtain a geometry that was prone to different types of shrinkage defects as to illustrate the features of the developed model. The designed shape casting is composed by blocks connected to the feeding system by different cross section dimensions. The aluminium alloys used in the model analysis, AlSi12 and AlSi7 (a short freezing and a long freezing alloy) were degasified before pouring in the sand mould.

Experimental results were obtained. Repeatability was observed in experimental results. The main defect found in AlSi12, short freezing alloy, was surface connected porosity, that decreased as the neck section size (feeding path) increased from 14 to 20 mm. Noticeable external sinks were absent. In AlSi7, long freezing, a sink in the top of the part, and an inner shrinkage porosity was observed (also more critical in the 14 mm section). Results were compared with simulations.

The expected shrinkage features are well described by the present model and illustrates the capability of the “defect” model to predict the key macro-phenomena of interest to the foundry industry. The numerical results reproduce the characteristic shrinkage defects profiles observed in the experimental results and also agree quantitatively with the experimentally measured porosity levels.

Samenvatting

In voorliggend proefschrift wordt een nieuw driedimensioneel model ontwikkeld, dat in staat is het ontstaan en de kenmerken van slinkdefecten in gietstukken expliciet te voorspellen, in functie van de wisselwerking tussen continuüm fenomenen, het stromen van vloeibaar metaal langs vrije oppervlakken, warmte transport en stollingsfenomenen, en dat voor complexe driedimensionele geometrieën. Er wordt een model ontwikkeld op fysische basis voor de beschrijving van het ontstaan van slinkholtes, dat in staat moet zijn rekening te houden met de verschillen tussen het stollingsgedrag van uiteenlopende legeringen, waarbij enerzijds de afkoeling een smalle randlaag laat stollen, alsook van legeringen die bij afkoeling stollen met een brijachtige consistentie en een lang stollingsinterval vertonen. Het model moet in staat zijn de hoeveelheid en de lokalisatie van de interne en externe slinkdefecten te voorspellen.

In het voorgestelde model gaat men ervan uit dat het volumetekort tengevolge van krimp enkel gecompenseerd kan worden door de volgende twee fenomenen: een inzakking van het buitenoppervlak van het gietstuk of de vorming van interne porositeiten, die ofwel aan het buitenoppervlak ofwel in het inwendige van het gietstuk starten. Zo lang het metaal zich na het gieten nog in vloeibare toestand bevindt, wordt dankzij de zwaartekracht het krimpen van het stollend metaal aangevuld met vloeibare fase vanuit de top van het gietstuk dankzij de zwaartekracht. Op een bepaald ogenblik begint een laag vast materiaal te groeien vanaf het oppervlak van de gietvorm naar binnen toe, waarbij een zone vloeibaar materiaal omsloten wordt. Om het optredende massatekort door krimp ten opzichte van de vloeibare fase te compenseren, moet er een materiaalstroom gegenereerd worden doorheen de stollende laag. Deze vloeistofstroom gebeurt tussen de groeiende dendrieten en ondervindt daardoor een toenemende graad aan wrijving, die resulteert in een drukverschil over de stollingslaag heen. Dat drukverschil kan een reeks problemen veroorzaken tijdens het stollingsproces van een gietstuk.

In het voorgestelde model wordt ervan uitgegaan dat er vloeibare legering vanuit het buitenste oppervlaktegebied door capillariteit kan weggezogen worden, wat bijzonder waarschijnlijk is bij legeringen met een groot stollingsinterval. In deze gevallen zal dan de uitwendige oppervlakte van het gietstuk inzinken ten einde de inwendige krimp op te

vangen. Anderzijds kan ook vloeibaar metaal vanuit stomphoekige gietvormlocaties weggezogen worden bij legeringen met een kleiner stollingsinterval, wat resulteert in een inwendige porositeit die uitgaat van het buitenoppervlak van het gietstuk en er tevens mee verbonden is. In legeringen met een kort stollingsinterval kunnen deze mechanismen echter reeds in een vroeg stadium uitgeschakeld worden, ten gevolge van een versnelde stolling aan de buitenste oppervlakken van het gietstuk. Indien geen enkel van de bovenvermelde mechanismen plaats grijpt, kunnen er inwendige porositeiten gevormd worden.

In voorliggend model wordt een element dat voldoet aan één van de boven beschreven voorwaaarden beschouwd als een element met vrij oppervlak. Een element met vrij oppervlak is een element waarin geen wet van behoud van massa wordt toegepast, zodat er vloeibaar metaal vanuit het element kan wegvloeien en aldus het gietstuk voeden. Indien een bepaald element een buurelement heeft dat geen metaal (geen materie) bevat, wordt dat element beschouwd als een element met uitwendig vrij oppervlak en een inzinking aan de oppervlakte van het gietstuk zal gevormd worden of een porositeit, verbonden met het oppervlak. Anderzijds, indien het element omringd wordt door elementen die metaal bevatten, ontstaat een inwendig vrij oppervlak, wat aanleiding zal geven tot de vorming van een interne porositeit.

Een continuïteitsvergelijking wordt toegepast om het transport van massa, energie en impulsmoment te beschrijven. Er wordt verondersteld dat de drijvende kracht voor de vloeistofstromen gedurende de stolling veroorzaakt wordt door het krimpen van het materiaal. Een bronterm van het Darcy type wordt opgenomen in de impulsmoment vergelijking om rekening te houden met de vloe weerstand ondervonden doorheen de brijachtige zone van het stollend materiaal. Een Volume of Fluid (VOF) model met vrij oppervlak wordt gebruikt om de krimpdefecten (oppervlakte-inzinkingen en inwendige slinkporositeiten), waarbij rekening wordt gehouden met het behoud van massa in het gietstuk. Door middel van een koppeling tussen de voedingsstroom, de druk en de stollingskinetiek wordt er een volledige methodologie opgebouwd, die toelaat slinkdefecten te beschrijven en bovendien de mogelijkheid heeft een dynamische slinkgeometrie in het gietstuk en in de aansneden te beschrijven.

De numerieke benadering van het probleem maakt gebruik van een compatibele set van eindige elementen procedures, met uitbreiding naar een ongestructureerd rooster. De implementatie van het model wordt in de thesis beschreven, samen met het testen van het model en een experimentele validatie ervan.

Ten einde de mogelijkheden en karakteristieken van het ontwikkelde model te illustreren worden er een aantal theoretische simulaties met een eenvoudige geometrie uitgevoerd. Deze simulaties tonen het ontstaan van de typische kenmerken van defecten die met slinkfenomenen gerelateerd worden. Ten einde de variabele morfologie van deze defecten duidelijk zichtbaar te maken, werd het gedrag geanalyseerd en vergeleken van twee legeringen met een binaire eutectische constituent, de ene met een kort stollingsinterval (klein temperatuurverschil tussen T_{liq} en T_{eu}) en de andere met een groot stollingsinterval (groot temperatuurverschil tussen T_{liq} en T_{eu}).

De resultaten tonen aan dat inwendige of uitwendige slinkdefecten optreden, afhankelijk van de grootte van het stollingsinterval van de legering. Het model toont aan dat legeringen met een kort stollingsinterval een grotere neiging vertonen voor de vorming van inwendige krimpporositeiten dan deze met een groot stollingsinterval, waarbij de slink optreedt onder de vorm van inzinkingen van het buitenoppervlak.

Ten einde de invloed van de in aanmerking genomen parameters van het model te evalueren, werd een eenvoudige proefopzet ontwikkeld, “cup test” genoemd, waarop de corresponderende numerieke simulaties werden uitgevoerd. Het doel van deze proeven was veelvuldig: een parametrisch bereik te identificeren voor de permeabiliteitscoëfficiënt (K_0); een criterium vast te stellen van kritische druk P_{crit} voor porositeiten, om deze dan te kunnen gebruiken voor de simulatie van complexe gietstukken; het analyseren van de invloed van het stollingsinterval en van de roostergrootte op de voorspelling van slinkdefecten.

Twee typische aluminium gietlegeringen werden gekozen, AlSi7 en AlSi12, waarbij kan gesteld worden dat de eerste legering (AlSi7) een lang stollingsinterval vertoont, terwijl de tweede legering nagenoeg de eutectische samenstelling heeft en dus een kort stollingsinterval. Op basis van numerieke resultaten was het duidelijk dat de permeabiliteit een belangrijke invloed heeft op de vorming van macroporositeiten en slinkholtes, zoals te

verwachten was. Bij een hoge permeabiliteit kan het vloeibare metaal voldoende gemakkelijk naar de stollingsgebieden vloeien om aldus een inzinking van de hogere gebieden te vermijden, ofwel, zoals in het geval van de legeringen met een groot stollingsinterval, om het inzakken van de wanden te vermijden. Bij lage permeabiliteiten echter is de toevoerstroom vanuit het hoger gelegen niveau in belangrijke mate beperkt, wat resulteert in een diepere inzinking in de top van de AlSi12-legering en bij de legering AlSi7 komt dat tot uiting in het uitzakken van de wanden. De impact van de initiële druk was zeer beperkt. Zodra de initiële druk een bepaalde waarde bereikt, worden de resultaten van de simulatie ongevoelig voor deze parameter.

Er werden experimentele stukken vervaardigd, uitgaande van gietvormen die bekend zijn voor het veroorzaken van verschillende types van slinkdefecten. Voor elke legering kon er na stolling een verschillende topgeometrie waargenomen worden. In het geval van de AlSi12-legering vertoont het bovenoppervlak een diepe inzinking, terwijl bij de AlSi7-legering een veel vlakker oppervlak optreedt. Ook een zekere graad aan inwendige porositeit wordt bij de twee legeringen waargenomen, waarbij de porositeit geringer en uniformer verdeeld is bij de AlSi7-legering.

De experimentele en numerieke resultaten worden met elkaar vergeleken ten einde de best passende parameterwaarden te verkrijgen. Het werd spoedig duidelijk welk parameterbereik het meest geschikt was om de experimentele waarnemingen te beschrijven.

Een andere proefopzet werd ontworpen: de “3-D complex shape”: een driedimensionele complexe gietvorm voor numeriek en experimenteel onderzoek. Bij het ontwerpen van de geometrie was het de bedoeling een reële gietsituatie te reproduceren, met een gietvorm bestaande uit het gietstuk en de toevoerkanalen, waarbij de geometrie zo eenvoudig mogelijk werd gehouden om beter in staat te zijn de variabelen te identificeren die rechtstreeks verantwoordelijk zijn voor de slinkdefecten tijdens het voeden van het gietstuk. Een andere vereiste was het verkrijgen van een geometrie die gemakkelijk aanleiding kan geven tot de verschillende soorten slinkdefecten, ten einde de eigenschappen van het ontwikkelde model op de voorspelling ervan te illustreren.

Het ontworpen gietstuk bestaat uit een reeks blokken die met elkaar verbonden zijn via aansneden met verschillende dwarssectie en verschillende vormen. De aluminiumlegeringen gebruikt voor de modelanalyses zijn AlSi12 en AlSi7, respectievelijk met een kort en een lang stollingsinterval. Deze legeringen werden gesmolten en na ontgassing gegoten in een zandvorm.

Uit de verkregen resultaten kon worden vastgesteld dat er een goede reproduceerbaarheid was. Het belangrijkste defect dat in de legering AlSi12 (met kort stollingsinterval) vastgesteld werd, was een met het oppervlak verbonden porositeit, die echter verminderde wanneer de vierkante dwarssectie van de aansnede van 14 naar 20 mm opgedreven werd. Er waren geen merkbare slinkfenomenen aan de buitenkant van het stuk. Bij de AlSi7-legering met een lang stollingsinterval werden een inzinking aan het bovenoppervlak van de vorm en inwendige porositeiten vastgesteld, dat gebeurde in belangrijkere mate bij een aansnede met vierkante sectie van 14 mm zijde. De resultaten werden vergeleken met de simulaties.

De te verwachten karakteristieken van de slinkfenomenen worden door het voorgestelde model steeds goed beschreven. Zij illustreren meteen ook de capaciteit van het hier ontwikkelde “defectenmodel” om de belangrijkste macroscopische fenomenen te voorspellen die van belang zijn voor de gieterijen. De numerieke resultaten beschrijven en reproduceren goed de karakteristieken van de slinkdefecten die bij de experimenten worden waargenomen en komen ook kwantitatief goed overeen met de gemeten niveau’s van porositeit in de experimentele stukken.

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CHAPTER 1

INTRODUCTION

“...The shortest distance between raw material and a finished part is a casting...”

Cook G., Engineered Castings.

1.1 Casting

Metalcasting represents the shortest route from the design of a part to its production. The molten metal is cast in a mould or die, which on solidification provides the part with its virtually definitive shape. A very attractive feature of casting processing is the possibility of manufacturing very complex products, which are very difficult or even impossible to produce by other means, with minor machining and with a minimum waste of material. The major advantages of this process are:

- almost no restrictions on complexity of shapes, contours, internal passages, undercuts, etc;
- ability to distribute metal where needed and to minimize weight in other sections;
- ability to cast a complex component as one piece rather than producing several parts that have to be assembled;
- ability for producing attractive complex contours for appearance purposes.

Castings are used in extremely wide and diverse fields. They range in weight of a few grams to several hundred tons, dimensions from millimetres to several meters. They go from decorator's trinkets to critical bridge structural parts. Shapes can be as simple as small bars or as complex as engine blocks or diesel engine heads.

Traditionally, casting process development is an inherent trial and error workflow. Design and engineering departments develop the guidelines for building a component mainly based on previous experiences. Although the foundry aims to manufacture the components in the desired quality, the initial casting trials of new prototypes often fail due to design inability.

It has been estimated that about 90% of the defects in components are due to mistakes in design and only 10% are due to manufacturing problems and the costs to change the design can increase ten-fold in every step of the design and manufacturing process [Louvo, 1997]. Hence, all the methods and tools used to ensure the success of the design will significantly affect the total manufacturing costs. Computer simulation can be the answer as a quick and effective tool in designing for the more and more complex castings and increased qualitative

requirements, with reduction or even elimination of time consuming tests and trial and error tuning.

Numerical simulation has been proving that, at the design stage, it can give important answers in analyzing the process and predicting the defects that may occur leading to process optimization [Gremaud, 2004; Kapturkiewicz, 2005]. Starting with the original design, a computer model is used to simulate the casting process. Given a set of defect models, defects can be predicted that suggest modifications to the original design. After several iterations of this *design cycle* an optimum design, free of defects should be produced, Figure 1.1.

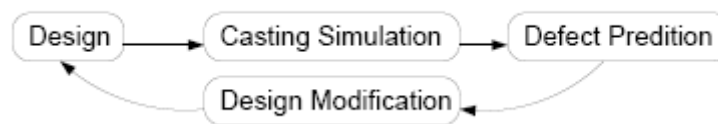


Figure 1.1: Process Optimization.

Obviously, the performance of this design cycle is based on the accuracy of the casting simulation and the validity of the defect models.

During the shape casting of most metals, cooling of the liquid phase and subsequent solidification is usually accompanied by a reduction in specific volume. If the shortfall in volume is not compensated by the feeding of additional metal then shrinkage porosity defect will develop.

Numerical modelling of shrinkage porosity in shape castings plays an important role when producing components of high integrity. High integrity castings means that all external geometric features are within the specific tolerance, there is no external evidence of defects and cut samples do not exhibit internal porosity.

The problem with solidification-based processing from a modelling perspective is that it involves the interactions among a wide range of phenomena: heat transfer, solidification and fluid dynamics (feeding flow and free surfaces). The promise has been that as we model physical processes closer to reality, the simulation becomes more accurate and the defect model more clear and precise. However, this promise comes at a price. First, as the model

improves it becomes increasingly sensitive to the thermophysical data. Often these data are difficult to obtain and therefore several new experimental techniques need to be developed. Second, as the mathematics becomes more complex there is a need to either develop efficient solution algorithms or invest in more powerful computer resources. It is the balance of all these factors that will result in a successful numerical application.

The initial drive of process modelling efforts was to produce software tools that only analyzed the solidification behaviour by heat conduction. The challenges evolved from the development of both basic algorithms and software tools, which facilitated the analysis of complex three-dimensional shapes. During the 1980s, a number of commercial codes began to emerge based upon conduction only. They often included empirical models for the evaluation of shrinkage defects based upon some relations of the local temperature gradient, e.g., the Niyama criterion [Niyama, 1981].

Despite the enormous progress in algorithms based on both finite element and control volume or finite volume approaches [Cross, 1993], most programs still use empirical formulae to predict defects in castings. Recently, due to the development of computer technology, an effort is done to predict casting defects directly as a consequence of the physical phenomena's that are involved. A modelling approach based on an improved description of the physical processes has become a more realistic and practical straightforward option.

1.2 The physics of shrinkage related defects

“...During freezing, liquid surges through the dendrite forest to feed the volume contraction on solidification, washing off branches, cutting flow paths, and polluting regions with excess solute, forming segregates. In those regions cut off from the flow, continuing contraction causes the pressure in the residual liquid to fall, possibly becoming negative (as a tensile stress in the liquid) and sucking in the solid surface of the casting. This will continue until the casting is solid, or unless the increasing stress is suddenly dispelled by an explosive expansion of a gas or vapour (shrinkage) cavity. The surface sinks are halted, but the internal defects now start...”

J. Campbell: Castings, Butterworth-Heinemann, 1991.

In a solidifying casting the density differentials requires the melt to move towards the solid front; therefore a velocity field is induced in the melt. This flow can have several impacts on the solidifying material: changing the solidified composition in alloys that affects the mechanical properties of the cast, changing the final shape, producing porosities which have a negative impact on mechanical properties such as ductility, dynamic properties and fatigue life [Campbell, 1991].

A positive pressure gradient from the outside to the inside of the casting will help to ensure that the feed material travels along the flow path into those parts of the casting experiencing shrinkage. The feeding flow is driven by the positive pressure such as atmospheric pressure and/or the pressure due to the hydrostatic head of metal in the feeder. The other part of the driving force for flow is the negative pressure generated by shrinkage. All of these driving forces happen to be additive; the flow of feed metal is caused by being pushed from the outside and pulled from the inside.

During the solidification of a casting, the gradual spread and growth of the solid, often in the form of a tangled mass of dendrites, presents increasing difficulties for the passage of feeding liquid. As the freezing liquid contracts to form the solid, the pressure in the liquid

falls, causing an increasing pressure difference between the inside and the outside of the casting. Such phenomena provide the driving force for the initiation and growth of volume defects such as porosity and surface sinks on castings.

A fall in internal pressure may cause mainly two problems:

- liquid may be sucked from the surface, Figure 1.2a). This is particularly **likely in long-freezing-range alloys**, or from re-entrant angles in **shorter-freezing range alloys**, Figure 1.2b), resulting in porosity initiated from, and connected to the outside;
- internal porosity may be nucleated, Figure 1.2 b).

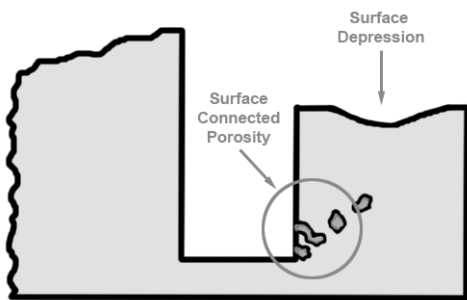
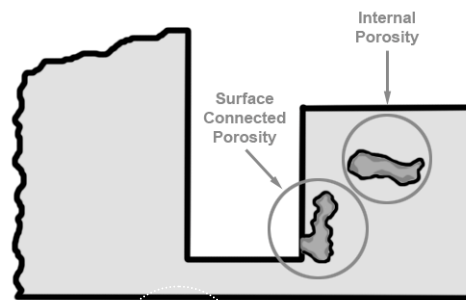


Figure 1.2: a) Long freezing aluminium alloy;



b) Short freezing aluminium alloy.

In shrinkage defects that are open to the atmosphere, the shrinkage is compensated by atmospheric gasses, a process that is independent of the gas content of the metal and which does not require gas pores nucleation and growth. On the contrary, closed shrinkage defects correlate well with the development of a critical internal stress (depression) at which some particular nuclei, or surface puncture, can be activated at one or more points in the casting. Feeding is then stopped at such a location, and pore growth starts.

In most cases the real situation is somewhere between these extremes, with castings displaying some internal porosity, together with some other parts of the casting surface displaying slight sinks.

Key points

In a long freezing material the free surface will be able to feed the casting much longer, due to the mushy solidification, and eventually most of the shrinkage will be compensated by the movement of the outside surface, external defects, Figure 1.2 a).

When considering a short freezing, the material of the outside layers quickly solidifies and feeding through free surface movement is soon impossible. Only from some re-entrant angles, connected to the free surface, this mechanism may still be activated. In these points material cools later and can still be sucked in, resulting in a porosity that is connected to the surface. When no more feeding from outside is possible the pressure quickly drops and the criteria for a pore to form are met, Figure 1.2 b).

1.3 Literature review

Simulation of shrinkage-related defects in shape castings have been extensively studied because of its potential contribution to quality improvement of cast products. In the past fifty years, especially in the recent twenty years, research efforts have been made to predict these defects with the help of computer simulation. These studies can be classified in the following approaches:

- Modulus and isothermal time method: determines the areas that solidify last.
 - Modulus method
 - Equisolidification thermal method
- Criteria function method: calculates parameters to characterize resistance to interdendritic feeding, delivering a critical value for porosity formation.
 - Niyama criterion
- Thermal volume models: directly simulates the formation of porosity by mathematically solving the heat transport and mass conservation.
- Thermodynamic models: model the shrinkage induced feeding fluid flow.
 - Microporosity model
 - Shrinkage model

The important results of these studies are reviewed in the next paragraphs.

1.3.1. Modulus and isothermal time method

1.3.1.1. Modulus method

The modulus method is based on Chvorinov's rule, [Chvorinov, 1940], the solidification time, t of a casting area is proportional to the square of its volume to area ratio, V/A , named modulus:

In equation (1.1) B is a factor that depends on the thermal properties of the metal and mould material. The rule simply states that under the same conditions, a casting with large surface area will cool more rapidly than one with a small surface area and the same volume.

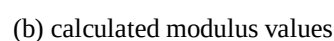
$$\frac{A_{riser}}{V_{riser}} < \frac{A_{part}}{V_{part}} \quad (1.2)$$


Figure 1.3: Shrinkage prediction by Modulus Method [Neises, 1987].

1.3.1.2. Equisolidification time method

With the introduction of Finite Difference/Element methods to foundry field, isothermal time contours could readily be calculated [Henzel, 1965; Jeyarajan, 1978; Iwahor, 1985]. It became possible to identify the last region to solidify “hot spots” in a casting and assuming that shrinkage cavities will be located in those regions. The principles of the calculations are well established and the results calculated are in good agreement with the corresponding experimental results in showing the last solidification area, Figure 1.4, [Iwahor, 1985].

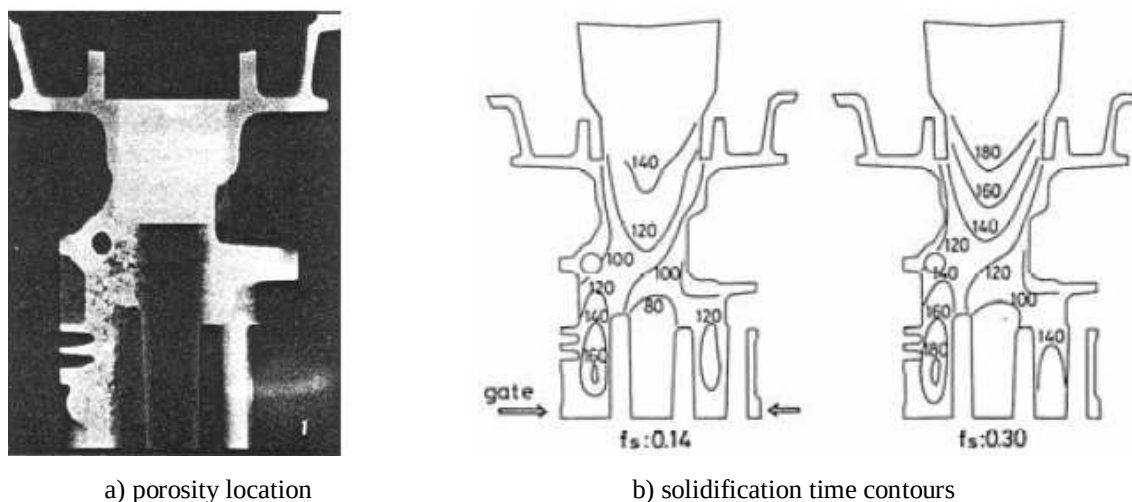


Figure 1.4: Porosity prediction of an engine block casting in AlSi alloy by equisolidification time method [Iwahor, 1985].

The deficiency of the modulus and equisolidification time method

To date, the determination of the areas that solidify last can be successfully carried on either by the modulus calculation or isothermal time calculation based on numerical simulation of heat transfer. In estimating solidification sequence, the latter is more accurate than the former, because modulus calculation does not take into account the mould temperature variation and the metal material physical properties. Therefore, the numerical simulation of heat transferring represents currently an important application of computer simulation in foundry industry. But both methods have their limitation in predicting shrinkage related defects, since they do not consider factors such as interdendritic feeding and gas evolution, which govern separately or cooperatively the formation of such defects.

1.3.2. Criterion function method

Thermal parameters used for criterion function method

Due to the inefficiency of the modulus and isothermal time method in predicting centreline and dispersed porosity, the criterion function approach has received considerable attention in shrinkage defects prediction. These criteria reflect the limiting conditions of interdendritic feeding. They are associated with thermal parameters, such as local temperature gradient G , cooling rate R , solidification velocity V_s and local solidification time t_f . A combination of these parameters, which can be easily obtained from the numerical solutions of solidification heat transfer, is often applied.

Temperature gradient, G , and other existing criteria

The importance of temperature gradient was first proposed by Bishop (1951) and developed by Niyama (1981), into a computer simulation method. This criterion gives information directly related to interdendritic flow. Therefore, it can predict centreline porosity more precisely than the isothermal time method, Figure 1.5.

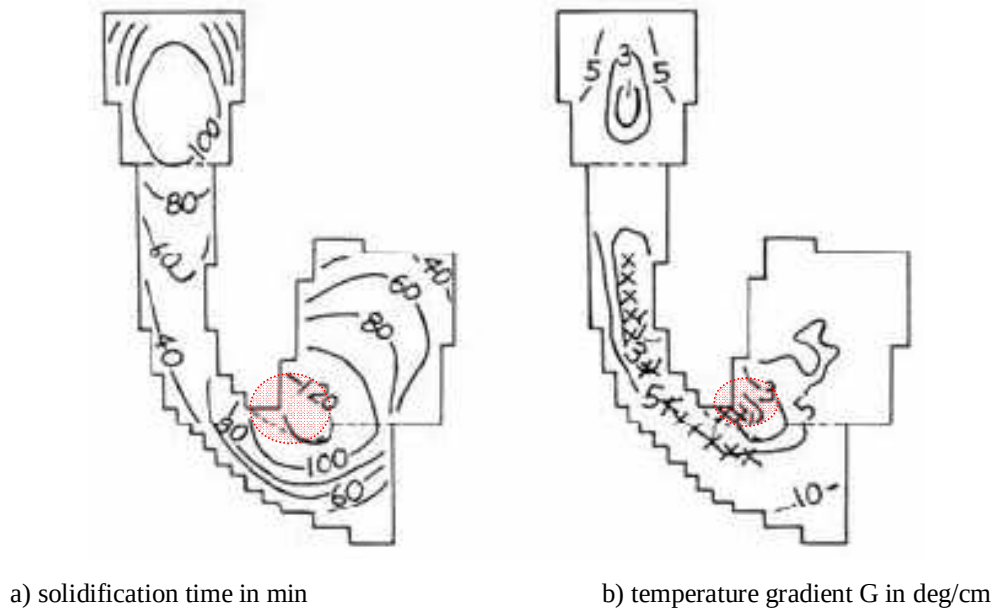


Figure 1.5: Comparison of G and isothermal time method in predicting shrinkage [Bishop, 1951].

The existing thermal parameter criteria proposed in literature so far, including temperature gradient G , are listed in Table 1.1.

Table 1.1: Thermal parameters based criteria for porosity prediction.

Criterion	Submitter	Time of publication
G	Bishop et al.	1951
G/V_s	Davies	1975
$1/V_s^n$	Khan	1980
$G/R^{1/2}$	Niyama et al.	1982
G/V_s	Lecomte-Beckers	1988
$G^{0.33}/V_s^{1.67}$	Lee et al.	1990
$G^{0.38}/V_s^{1.62}$	S.T.Kao et al.	1994
$1/t_s^m V_s^n$	F.Chiesa	1998

All these criteria can be reduced to the form of G^x/V_s^y (x varies over the range 0~2 and y varies over the range of 0.25~1), among which the Niyama criterion that can be reduced to G/V_s is a representative one.

1.3.2.1. The Niyama criterion

Niyama et al. (1982) found that the critical temperature gradient was inversely proportional to the square root of the solidification time, Figure 1.6.

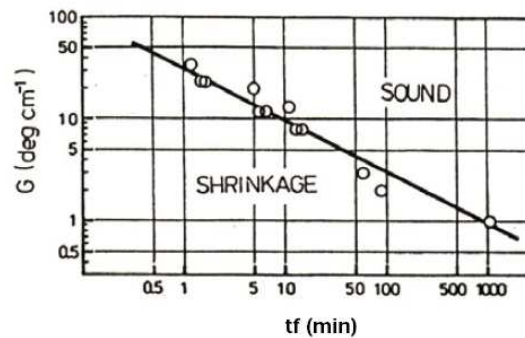


Figure 1.6: The relation between the experimentally determined critical temperature gradient G and the calculated solidification time t_f [Niyama, 1982].

Therefore, they proposed to use $G/R^{1/2}$ at the end of solidification as a criterion for porosity prediction. This criterion was justified by Darcy's Law, so that it included the physics behind the difficulty of providing feed liquid in the last stages of solidification when the interdendritic liquid channels are almost closed.

The authors have proposed a critical value of $1.0 \text{ (deg}^{1/2} \text{ min}^{1/2} \text{ cm}^{-1}\text{)}$, and its effectiveness has been verified with steel castings [Minakawa, 1985]. For each point in a casting, the Niyama criterion is evaluated at the end of solidification. Niyama et al. define the end of solidification as the time when the temperature first reaches or drops below the solidus temperature (T_s).

The advantage of these criteria functions is that they provide a straightforward means of assessing the influence of various casting parameters such as thermal gradient, cooling rate, and solidification time on porosity. They are also easy to implement and quick to run in process heat-transfer models. The Niyama criterion has been widely integrated into current existing computer software to relate the output of the numerical heat transferring calculations (temperature gradient, solidification time, etc.) to empirical findings on porosity [AFS, 1994; Magmasoft, 1995; Hicass, 1998; AdStefan3D, 2003].

Key point

Regions in which porosities or cavities are due to the presence of hot-spot are easily spotted, other regions, where interdendritic cavity defects or sink surface occurs, cannot be predicted.

Also they are insensitive to varying hydrogen concentration (in aluminium alloys) and generally present poor quantitative capability.

1.3.3. Thermal volume models

Beginning from the 1980's, there have been attempts to predict shrinkage defects quantitatively by direct numerical simulation. These models solve the heat transport problem and attempt to predict defect locations through simple change in volume calculations based on mass conservation, thus avoiding rigorous flow analysis of the molten metal during solidification.

The solid fraction is thought to be the key parameter in deciding the feeding mode for these models, where the solid fraction f_s , is the solid phase volume fraction, $f_s = v_s/v$ of an element. Imafuku and Chijiwa (1993) calculated the shapes of shrinkage cavities based on this principle. They categorized shrinkage defects as macroscopic and microscopic cavities, named shrinkage and porosity respectively. The mechanism of the formation, and hence the predicting methods for the two classes of defects, were said to be different. The liquid flow induced only by gravity was considered to be the cause of the formation of a shrinkage cavity in an isolated semi-solid region with low solid fraction, namely $f_s < f_{sc}$, Figure 1.7a), where f_s and f_{sc} represent solid fraction and the critical solid fraction, respectively. Solidification shrinkage in an isolated semi-solid region with high solid fraction, i.e. $f_s > f_{sc}$, Figure 1.7b), was considered to be the origin of porosity. This model assumes that liquid metal free surface is flat and normal to the gravity vector, the volume of shrinkage cavity is equal to the volume contraction of the metal, macroscopic fluid flow exists as long as the fraction solid, f_s is less than a critical fraction.

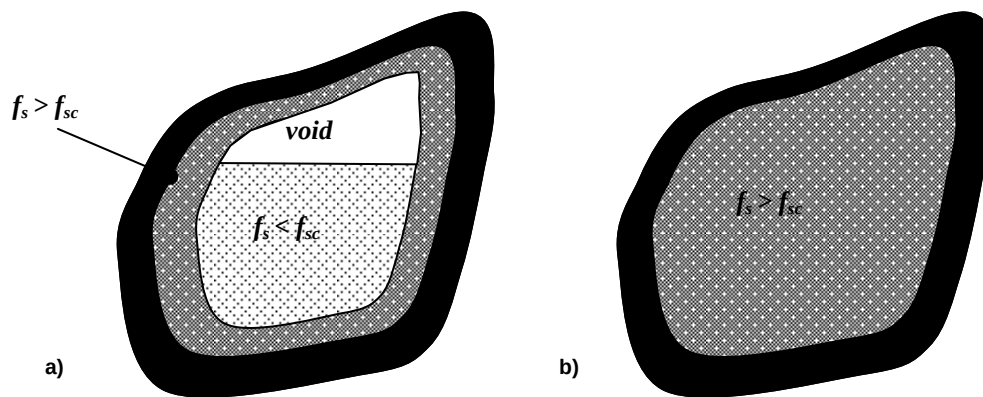


Figure 1.7: Typical casting simulation domain a) shrinkage porosity; b) microporosity.

The potential for the formation of a shrinkage cavity is evaluated according to the following methodology.

When a unit volume of the casting changes phase from a completely liquid state to a solid state, the resulting volume fraction change is given by:

$$\beta = \frac{\rho_s - \rho_l}{\rho_l} \quad (1.3)$$

which is positive for metals that shrink upon solidification. Thus, when the liquid fraction of a unit cell "i" of volume v_i , in the discrete casting, changes by Δf_{s_i} over a time Δt , then the change in volume in the cell is given by:

$$\Delta v_i = -\beta \Delta f_{s_i} v_i \quad (1.4)$$

where

$$\Delta f_{s_i} = f_{s_i}^t - f_{s_i}^{t+\Delta t} \quad (1.5)$$

if there are "n" cells in a given pool, then the change in the volume of that pool at time t is given by:

$$dp = \sum_{i=1}^n \Delta v_i = -\beta \sum_{i=1}^n \Delta f_{s_i} \Delta v_i \quad p=1,2,3,\dots,\text{mpool} \quad (1.6)$$

The applicability of the mathematical model to practical problems was verified with steel castings, [Imafuku, 1983(2)].

A similar approach was used by Beech et al. (1998). Heat conduction in the casting and mould was coupled with calculation of the volume change because of solidification contraction for each isolated liquid region of the casting at any given time. The volume change was calculated by $\Delta v_i = \beta v_0 fsF$, where fs is the fraction of solid and F is the fluid fraction ($F = 0$ for an empty volume element is empty, $F = 1$ if the volume element is full). A partially occupied volume will have a F between 0 and 1.

Key point

These models rely on the boundary condition determination only as a result of thermal calculation. It is necessary to track the front liquid/solid and this depends on empirical assumptions. Although this approach can be quite useful for steels, the same doesn't apply for aluminium alloys.

1.3.4. Fluid flow models

In castings, shrinkage defects can take the form of internal porosity, interconnected porosity linked to a free surface or surface depressions (refer to Section 1.2, page 1).

While the hot-spot regions, where shrinkage cavities can be found, can be easily spotted using a simple thermal analysis, shrinkage quantification isn't so straightforward. Also this methodology can't predict the interconnect porosity or surface defects. Detailed mechanism for feeding deficiencies should be modelled to describe the formation of this type of defects.

The first models to consider feeding flow during solidification were the gas porosity models. Gas porosity presents a regular, rounded shape, is well distributed and is usually a result of the presence of hydrogen.

After a succinct analysis of gas porosity models, an overview of recent approaches to model shrinkage defects that include the modelling of feeding flow is presented.

1.3.4.1. Gas porosity (*Microporosity*)

Gas porosity isn't considered a shrinkage defect, although one of the mechanisms behind its formation is the pressure drop due to shrinkage. The models proposed to predict the gas porosity have allowed a different approach on shrinkage defects, since it considers the pressure drop due to shrinkage and the feeding flow.

Various approaches have been adopted to solve for the pressure field within the developing interdendritic network. These range in sophistication from straightforward analytical expressions, derived on the basis of steady-state solidification conditions [Piwonka, 1966] to more realistic transient solutions, based on models describing flow through porous media, according to Darcy's Law [Darcy, 1856]. These models relate porosity formation to the local metal pressure and typically also consider the variation in hydrogen solubility together with a hydrogen mass balance.

A number of studies attempted to understand the phenomena of porosity formation and pore growth [Kubo, 1985; Ampuero, 1990; Zhu, 1990] and pore morphology [Nastac, 1999]. Most of these models solve the shrinkage with information obtained mainly from the thermal field and introduce a model for gas porosity.

The earliest prediction of gas microporosity distributions that is generally applicable to shaped castings was made by Kubo and Pehlke (1985).

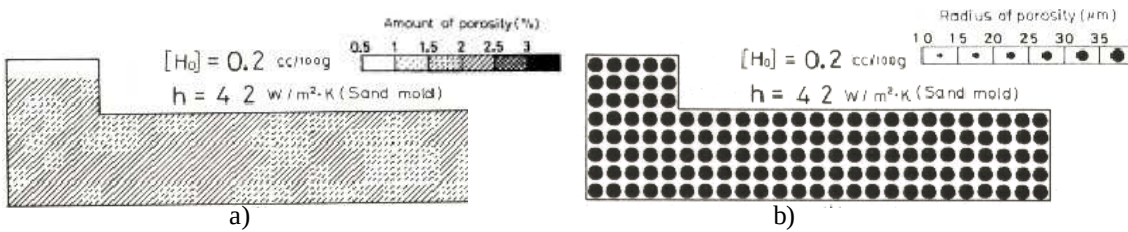


Figure 1.8: a) Calculated percentage porosity in Al4.5Cu plate castings b) and pore radius [Kubo, 1985].

Kubo and Pehlke (1985) presented a 2-D methodology for the prediction of gas microporosity distribution in shaped castings. In their study, the effects on porosity formation of both the hydrogen precipitation during solidification and the pressure drop due to the feeding resistance of the mushy zone were considered. The pressure drop during solidification regime was calculated only in the interdendritic-feeding regime using Darcy's law:

$$v = -\frac{K}{\mu} \nabla P \quad (1.7)$$

Where v is the average velocity, K is the permeability of the porous medium, μ is the shear viscosity ∇P is the pressure drop. The permeability was formulated based on the Carman-Kozeny model [Carman, 1937].

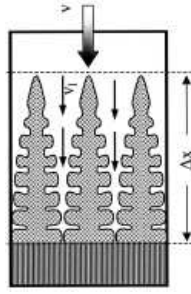


Figure 1.9: Schematic representation of 1-D columnar mushy zone.

Subsequently they substituted Darcy's equation for velocity in to the continuity equation (1.8) relating the reduction in volume due to shrinkage to the liquid feeding and pore growth:

$$\frac{\partial(\rho_s f_s - \rho f_l)}{\partial t} + \nabla(f_l v) + \frac{\partial f_g}{\partial t} = 0 \quad (1.8)$$

where f_l and f_p are the fraction liquid and porosity, respectively. If no pores are formed they are solved for the pressure and then checked whether sufficient supersaturation had occurred for nucleation. This was done by using the pressure of the gas inside the pore, P_g , as given by Piwonka and Flemings (1966):

$$P_g = P_m + P_\sigma \quad (1.9)$$

and the hydrogen evolution as:

$$f_g C_H^u = C_H^0 - C_H^l (f_s k_H + f_l) \quad (1.10)$$

where $P_\sigma = 2\sigma/r$, is the pressure due to surface tension. The initial pore radius, r , was assumed 1/2 of the SDAS (Secondary Dendrite Arm Space). C_H^l is the initial gas concentration within the liquid, K_H is the partition coefficient for hydrogen between solid and liquid. The hydrogen concentration on the liquid (C_H^l) and gas pressure (P_g) are related through Sievert's law as :

$$C_H^l = S\sqrt{P_g} \quad (1.11)$$

S is the hydrogen solubility in the liquid.

Kubo and Pehlke first calculated the change in fraction liquid. Then they solved equation (1.7) and (1.8) to determine the local metal pressure using an explicit finite differences approximation. Next they solve equation (1.9) to determine the gas pressure. To do this they assumed that the pore will nucleate on the solid/liquid interface of a dendrite and that the pore's diameter will equal the secondary dendrite arm spacing. With the calculated gas

pressure, they tested to see if any porosity would have formed using equation (1.10). After porosity is formed, then they use equations (1.7) and (1.8) to determine the liquid flow instead of the pressure. If flow is positive, they use equation (1.7) and (1.8) with equation (1.9) to determine P and P_g using the value of f_g from the previous time step. If the flux of liquid was negative, then the porosity was first computed using the pressure at the previous time step.

The liquid-feeding and mass-feeding regimes were neglected. The local pressure and porosity were computed in an uncoupled manner.

The methodology proposed by Kubo and Pehlke has been used with little change in numerous studies, such as those of Combeau and Rousset *et al.* (1995).

An extensive review of the research progress in microporosity modelling, from these early studies up to work done in 2000, is provided by Lee (2001).

1.3.4.2. Shrinkage defects

Suri and Paul (1993) simplified and extended the Kubo and Pehlke work to three dimensions, with shrinkage porosity predictions. The shrinkage model predictions are only based on thermal calculations. They need to set a critical solid fraction, f_{sc} , and look for regions where liquid is “fluid” enough to flow, $f_s < f_{sc}$ region (A) in Figure 1.10, surrounded by metal with higher solid fraction, f_{sc} , region (B) in Figure 1.10. Then shrinkage porosity forms and is computed to balance the volume shrinkage of such area.

The model depends on boundary condition defined by a critical solid fraction f_{sc} , obtained only from thermal analysis, to decide which type of defect will be computed, shrinkage or gas defects.

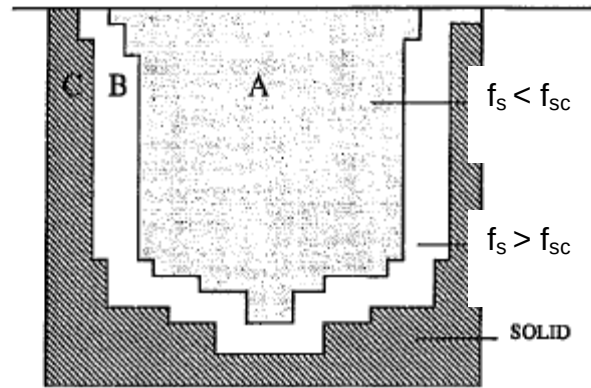


Figure 1.10: Typical casting simulation domain where a liquid pool (region A) is isolated [Suri, 1993].

Another recent 3-D model is presented by Pequet (2002). This approach couples a microporosity model based on Darcy's equation with macroporosity and shrinkage pipe predictions. They incorporate this into casting solidification simulation by superimposing a fine finite volume grid onto the coarser finite element mesh used for heat flow computations. They solve the governing equations of microporosity formation in the mushy zone and impose boundary conditions around this zone. To determine the boundary conditions, they should decide if each liquid region of the casting is connected to a free surface, surrounded by solid or surrounded by a mushy zone, Figure 1.11.

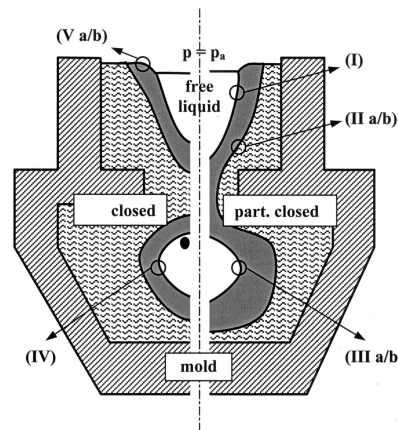


Figure 1.11: Boundary conditions applied at the boundary of the mushy zone for (I) the liquidus front of an open region of liquid, (II) the root of the mushy zone, (III) the liquidus front of a partially closed liquid pocket, (IV) the liquidus front of a closed liquid pocket, and (V) the free surface [Pequet 2002].

More recently, Sabau and Viswanathan (2002) provided a 3-D model for porosity prediction in hydrogen-aluminium alloy systems that augment a microporosity prediction model with

the ability to compute shrinkage porosity when feeding flow is cut off. Combining the Darcy's law with the equation for Navier-Stokes flow they obtain a momentum equation that is valid in all domain, both in the liquid region and in the mushy zone. The condition for interdendritic feeding is set to $f_s > f_{s_{coherency}}$ where $f_{s_{coherency}}$ is the coherency solid fraction.

The interdendritic liquid pressure during solidification decreases with the liquid fraction until the saturation of hydrogen point is reached. A pore nucleates and the pore fraction evolution is described by the hydrogen mass conservation and Sievert's law (1.11).

The condition for feeding cut-off is decided on a fraction solid threshold, defined as: $f_s = 1 - f_{eutectic}/2$, where $f_{eutectic}$ is the eutectic fraction of that alloy and they no longer solve for pressure or velocity in the region. When severe feeding deficiencies occur the pressure drop can reach the cavitation pressure for aluminium (at 750° $P_c = 10E-6$) [Handbook of Chemistry, 1989]. Once liquid pressure in cell reaches the cavitation pressure the feeding calculation stop and porosity will grow function of the shrinkage in that cavity.

Bounds et al. (2000) developed a 3-D code that predicts macroporosity misruns and pipe shrinkage in shaped castings. The flow model is based on an approach, single domain, developed by Chang and Stefanescu, (1994) for macrosegregation. They solve mixture Navier-Stokes and energy equations using an effective viscosity to account for the motion of solid in the melt below the coherency point. Only one set of equation to solve mass energy and momentum transport equations is used. The need to track the interface boundary is eliminated.

The model doesn't account for the gas content in the melt, but they account for model air flow in the mould and the rise of free gas pores in the liquid metal. They propose a model for predicting internal porosity, Figure 1.12a), and surface connected porosity Figure 1.12b). Internal porosity forms if the pressure drops below an arbitrary value and external porosity if the air can be drag of free surface.

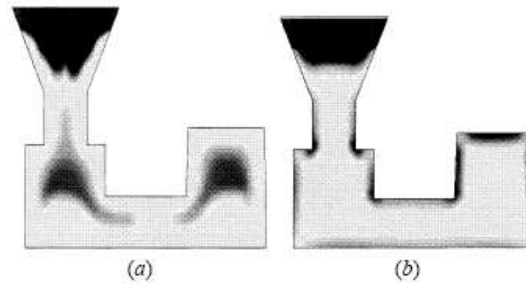


Figure 1.12: Predicted shrinkage a) short freezing alloy; b) long freezing alloy [Bound, 2000].

They show qualitative results for a two dimension model, Figure 1.12, but do not provide any quantitative shrinkage results, i.e., void fractions. Also there are no experiments to validate this model with regard to the factor that determines whether shrinkage porosity is either internal or surface connected or both.

Carlson (2003) presented a single-domain 3-D approach to determine pressure and feeding flow in the liquid as well as the mushy zone. The model assumes that each volume element in the casting is composed of some combination of solid metal (s), liquid metal (l), porosity (p), such that the volume fractions satisfy: $f_s + f_l + f_p = 1$.

This model uses a simplified momentum equation:

$$\nabla^2 v = \frac{f_l}{K} v + \frac{f_l}{\mu_l} \nabla P - \frac{f_l}{\mu_l} \rho_{ref} g \quad (1.12)$$

They reduce to Stokes' equation in the single-phase liquid region, where K becomes very large. Also, they assume that in the mushy zone, the left-hand side of equation becomes very small relative to the permeability term, and the equation then reduces to Darcy's law. By manipulating and combining this simplified equation with mass conservation, it is possible to derive a equation for the melt pressure, P . This assumption allows to be decoupled from momentum equation.

When porosity forms, the melt pressure at that location is forced to $P = P_p - 2\sigma/r$. This allows the continuity equation to be solved and determine the pore fraction. Note that in

regions that are completely surrounded by solid, forcing the pressure to $P = P_p - 2\sigma/r$, results in a very small growth of porosity, that isn't very realistic.

Recently [Carlson, 2006] they present a detailed model for microporosity- hydrogen diffusion.

Zhu et al (2006) performed experimental work with aluminium alloys with different contents of hydrogen. Measured porosity distributions in the test castings with low initial hydrogen content (0.053 cc/100 g or less) revealed porosity that was not detected by microporosity model. The reason for this prediction was due to the initial hydrogen content being so low that the critical supersaturation, for a pore to nucleate, was never reached within the residual liquid before complete solidification. This behaviour ultimately led to the development of a two-stage model to predict porosity: stage I occurring at fractions solid prior to liquid encapsulation (liquid feeding possible) and stage II occurring at fractions solid after liquid encapsulation (no liquid feeding possible). In the first stage, the volume fraction of porosity is calculated based on the reduced pressure, whereas, in the second stage, at fractions solid greater than the liquid encapsulation point, the fraction porosity will be determined by the size of the isolated pockets of liquid and the volumetric contraction coefficient of the alloy.

The f_{sc} is estimated using a correlation based on the Niyama parameter:

$$f_{sc} = 0.6271 + 0.047 \ln \left(\frac{G}{\sqrt{R}} \right) \quad (1.13)$$

1.3.4.3. Comparison of previous models

In all methodologies outlined, the location and severity of interdendritic cavity defects are predicted using methods based on thresholds for interdendritic liquid metal flows. These values are obtained from the heat transport model while the amount of gas porosity is (well) predicted using models that include fluid dynamics.

The approach to compute shrinkage defects based only on thermal analysis, doesn't predict regions, where interdendritic cavity or surface sinks defects form. These types of defects need a detailed model for mechanisms for feeding deficiencies in order to accurately be localized and quantified.

Only Bounds et al. (2000) proposed a model that explicitly calculates shrinkage defects as a result of deficiency in feeding flow. They present results for a 2-D numerical problem that illustrate the ability to compute internal and surface interconnected defects but actually no quantitative results were presented.

Key point

To date no methodology has been proposed to quantify the extent of shrinkage porosity, coupling internal (cavities) and external (surface connect or surface depression) shrinkage defects which occurs when solidification shrinkage cannot be compensated by feeding flow.

There are no validation experiments that are suitable to this model regarding to the factor that determines whether shrinkage porosity is either internal or surface connected or both.

1.4 Scope and objectives of this thesis

At the outset of this work, it is important to distinguish between the class of defects addressed. There has been a sustained research effort in the last decade to characterize the factors that control microporosity as outlined in previous section. The length scales of these phenomena are micrometers compared to component dimensions of millimeter-centimeter. Nevertheless, microporosity in castings can have profound effect upon their mechanical and fatigue properties. However, in this work we are concerned with defects, which are essentially shrinkage driven.

Among all the shrinkage related studies, this work aims to extend the scope of the above mentioned theories (Section 1.3.4) and develop a model for shrinkage driven defects to describe the extent of shrinkage porosity, its location and type, *ie.*, internal or surface connected, entirely as a function of the continuum physics employed, which to our knowledge has never been achieved before.

In the present model the volume deficit due to shrinkage can only be compensated by two phenomena: by depression of the outside surface or by creating internal porosity that can be started on the surface or in the interior of the casting. When the metal is still liquid after pouring, the shrinkage of the material is fed from the top driven by gravity. At some instant a solid layer will grow inwards from the mould interface, enclosing a liquid region. To compensate the mass deficit within liquid region, a flow has to be generated through the solidifying layer. This flow through the emerging dendrites will observe an increasing friction, resulting in a pressure drop across the solidifying layer. When the pressure drops below a certain critical pressure a pore will open. After the pore has opened the pressure inside the pore is considered to be constant. So the model should allow for calculation of free surface flow through a porous medium, driven by mass continuity and gravity. This flow should be coupled to the pressure to check if it has dropped below the critical pressure. For short freezing range alloys a solid skin forms at the mould-metal interface. Once the feeding path becomes obstructed, the pressure drop in the solidifying region triggers macroporosity formation. For long freezing range alloys, the mushy zone extends to the surface of the

casting. The air can be drawn into the casting through the semi-solid surface, and shrinkage may form at the hot spots on the surface.

The advantage of this approach is the direct coupling between the feeding flow and shrinkage defects. Unfortunately, quite powerful computer facilities are needed to perform the necessary calculations. Therefore, there is a need for accurate but also efficient formulations and implementations of shrinkage defects into numerical codes.

The aims of this work are:

- to present a physics-based model for shrinkage defects that capture the difference in solidification behaviour of skin freezing material and mushy freezing alloy by predicting location and extent of internal and external shrinkage;
- to incorporate this shrinkage defect model into a numerical formulation of casting process;
- to perfectly document the features of the model developed here, by performing a number of theoretical simulations that exhibit well known features of shrinkage related defects and perform sensitivity analysis;
- to design and test a casting geometry, prone to internal and external defects;
- to validate this new shrinkage defect model with experimental casting tests;
- to convince that including advanced shrinkage modelling into FD/FE casting simulations is not only possible and realistic from computational point of view but also necessary for the accuracy of predictions in order to better design castings avoiding and mastering the skin and internal shrinkage defects.

1.5 Layout of the thesis

This introduction is the **first chapter** of six. It includes a **literature review** where contributions that have been made to the field of solidification modelling with focus on modelling shrinkage related defects are presented. Its aim is to highlight problems and areas of weakness that need to be researched in this work. Given this direction, it outlines the scope and objectives of the thesis to provide a framework for remaining chapters.

The **chapters 2, 3 and 4** in this thesis closely follow the construction and testing of a computer model, the aim of this work, as represented in Figure 1.13.

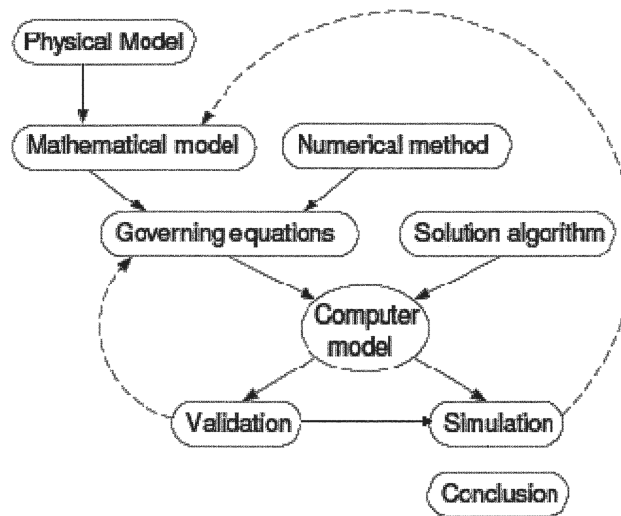


Figure 1.13: Construction of a computer model.

The construction of a computer model can be broken into several stages, starting with a **physical model** that is based upon a number of simplifying physical assumptions. These assumptions can be made in light of our understanding of the physical processes that are involved. From the physical model and a series of differential equations, a **mathematical model** is built, which is described in **Chapter 2**.

In a typical physical process the differential equations derived cannot be solved analytically but have to be solved numerically. Normally, the nature of the mathematical model would dictate the type of **numerical method** to be employed. A combination of the mathematical model and numerical model leads to a set of **governing equations**. Before these governing equations can be solved, a **solution algorithm** should be developed that can solve the equations quickly and correctly. **Chapter 3** examines the numerical methods to be used and describes the solution algorithms.

The developed computer model is tested in **Chapter 4**. Sensitivity of the computer model is then checked against known effects of solidifying metal by performing a number of theoretical simulations that exhibit well known features of shrinkage related defects. The effects of various parameters and control parameters upon the simulation are observed. This knowledge is used to characterize the performance of the model.

Once the computer model has been tested it can be used to perform real simulations. In **Chapter 5** the experimental work is described. The **simulations** are compared with experimental and the efficiency of the model is discussed.

Comments on the success and failure of the aims and objectives of this thesis are presented in **Chapter 6**. Any problems that have arisen are discussed and recommendations are provided for future work.

CHAPTER 2

MATHEMATICAL MODEL

This chapter presents a physics-based model for shrinkage defects that capture the difference in solidification behaviour of skin freezing material and mushy freezing alloy by predicting location and extent of internal and external shrinkage.

2.1 Physical model

In this chapter the developed 3-D model for shrinkage defects prediction is presented. The aim of this model is to capture the difference in solidification behaviour of long and short freezing materials. The shrinkage defects in short freezing materials tends to be internal, such as porosity, while in long freezing materials these defects tend to be external in the form of surface depressions.

A complete methodology that enables the possibility to show dynamic shrinkage geometry in the casting and feeding system is presented.

In the present model the volume deficit due to shrinkage can only be compensated by two phenomena: depression of the outside surface or by creation of pores. The mechanism to create these defects is indicated in Figure 2.1.

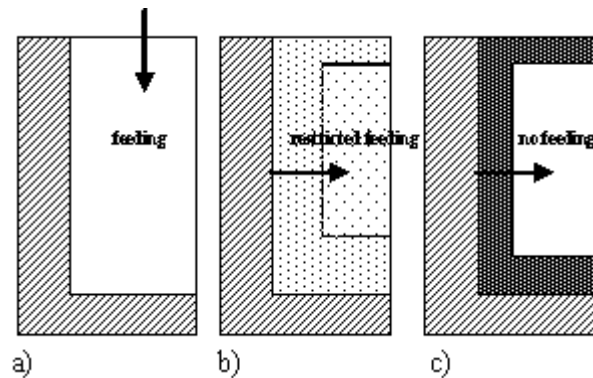


Figure 2.1: Mechanism for shrinkage defects.

When the metal is still liquid, after pouring, the shrinkage of the material is fed from the top and driven by gravity, Figure 2.1(a).

At some instant a solid layer will grow inwards from the mould interface, Figure 2.1(b), enclosing a liquid region. To compensate the mass deficit within liquid region, a flow has to be generated through the solidifying layer. This flow through the emerging dendrites will observe an increasing friction, resulting in a pressure drop across the solidifying layer. When the pressure drops below a certain critical pressure, a pore will open, Figure 2.1(c). After the pore has been opened the pressure inside the pore is considered to be constant.

2.2 Fundamental equations

a. Mass

The material deficit due to density increase, which is the case of most alloys, has to be compensated by metal flow that is described by the mass conservation equation:

$$\frac{\partial \rho}{\partial t} + \nabla(\rho u_i) = 0 \quad (2.1)$$

where u_i is the velocity vector and ρ is the material density.

In a scalar form this eq. (2.1) becomes:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho \cdot u)}{\partial x} + \frac{\partial(\rho \cdot v)}{\partial y} + \frac{\partial(\rho \cdot w)}{\partial z} = 0 \quad (2.2)$$

b. Momentum

The feeding velocities in the casting are determined from the momentum equation:

$$\rho \left(\frac{\partial u_i}{\partial t} + u_i \nabla u_i \right) = -\nabla P + \rho g_i + \mu \nabla^2 u_i + S \quad (2.3)$$

where P is the pressure, ρg_i is the body force and S is a loss term.

During solidification the convection and diffusion terms have a very small contribution. The velocities induced by shrinkage are very small and these terms can be $10^6 \sim 10^8$ times smaller when compared with the body force and pressure drop. The convection and diffusion terms being dropped, eq.(2.3) becomes simplified:

$$\rho \frac{\partial u_i}{\partial t} = -\nabla P + \rho g_i + S \quad (2.4)$$

It is assumed, that when solidification starts, a loss moment, S in eq. (2.4), is introduced.

This loss is modelled as flow through a porous medium, and thus can be approximated by Darcy's law. This Darcy term is represented by:

$$S = -\frac{\mu}{K} u_i \quad (2.5)$$

where K is the permeability. K reflects the resistance of the already solidified metal to the feeding flow. K depends on the amount of solid fraction, f_s , and can also account for the solidification morphologies.

In this study the Kozeny-Carman relation for permeability was used:

$$K = K_0 \frac{f_s^2}{(1 - f_s)^3} \quad (2.6)$$

where K_0 is the permeability coefficient that is typically function of a characteristic dimension and solidification morphology.

Expressing eq. (2.4) in the three directions we have:

$$\frac{\partial}{\partial t}(\rho u) = -\frac{\partial P}{\partial x} + \rho g_x - \frac{\mu}{K_x} u \quad (2.7)$$

$$\frac{\partial}{\partial t}(\rho v) = -\frac{\partial P}{\partial y} + \rho g_y - \frac{\mu}{K_y} v \quad (2.8)$$

$$\frac{\partial}{\partial t}(\rho w) = -\frac{\partial P}{\partial z} + \rho g_z - \frac{\mu}{K_z} w \quad (2.9)$$

c. Energy

The heat transfer during solidification is governed by the law of energy conservation, eq.(2.10). The heat is transported by conduction and convection.

$$\frac{\partial}{\partial t}(\rho C_p T) + \nabla(\rho C_p u_i T) = \nabla(k \nabla T) + S \quad (2.10)$$

C_p is the specific heat and k is the thermal conductivity.

To account for the latent heat lost during solidification, the latent heat is included into the energy equation, by the “ S ” term in eq.(2.10). Typically “ S ” is a function of the fraction solid:

$$S = \rho L \frac{\partial f_s}{\partial t} \quad (2.11)$$

where L is the latent heat of fusion of the alloy. Eq. (2.10) is then written:

$$\frac{\partial}{\partial t}(\rho C_p T) + \nabla(\rho C_p u_i T) = \nabla(k \nabla T) + \rho L \frac{\partial f_s}{\partial t} \quad (2.12)$$

Moving the second term from the right end side to the left of eq. (2.12) gives:

$$\rho \left(C_p - L \frac{\partial f_s}{\partial t} \right) \frac{\partial T}{\partial t} + \nabla(\rho C_p u_i T) = \nabla(k \nabla T)$$

and considering:

$$C_a = \left(C_p - L \frac{\partial f_s}{\partial t} \right) \quad (2.13)$$

where C_a is called the modified specific heat, and accounts to the loss during solidification.

Eq. (2.12) becomes:

$$\rho C_a \frac{\partial T}{\partial t} + \nabla(\rho C_p u_i T) = \nabla(k \nabla T) \quad (2.14)$$

When metal temperature lies within the solidification range C_a is calculated as in eq. (2.13), otherwise $C_a = C_p$. In a scalar form this equation (2.14) is written as:

$$\rho C_a \frac{\partial T}{\partial t} + \underbrace{\rho C_p \frac{\partial}{\partial x}(uT) + \rho C_p \frac{\partial}{\partial y}(vT) + \rho C_p \frac{\partial}{\partial z}(wT)}_{\text{convection}(cv)} = k \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) \quad (2.15)$$

To solve eq. (2.15) a relationship between casting temperatures and the solid fraction should be specified. In theory, the fraction of solid should be calculated from the nucleation and growth of metal dendrites. In practice, this simulation is too complex. Instead, a number of approximations may be used to calculate f_s . In this work the solid fraction varies linearly between the liquidus and solidus temperature, which yields:

$$\begin{aligned} f_s &= 0 & T &> T_l \\ f_s &= \frac{T_l - T}{T_l - T_s} & T_l &< T < T_s \\ f_s &= 1 & T &< T_s \end{aligned} \quad (2.16)$$

where T_{liq} and T_{sol} are the liquidus and solidus temperature, respectively.

d. Free surface treatment

The profile of any free surface (external or internal) is described by an F function. This function is similar to the function used in VOF method [Nichols, 1980] for free surface tracking. In this method, the fluid is represented by a step function. Since this function should be conserved as it is convected with the fluid, the time dependence of F is governed by the following equation:

$$\frac{\partial F}{\partial t} + \nabla(Fu_i) = 0 \quad (2.17)$$

Physically $\frac{\partial F}{\partial t}$ represent the amount of liquid that flows from the free surface element to compensate shrinkage.

When averaged over the cells of a spatial mesh, the average value of F in a cell is equal to the fractional volume of the cell filled by the metal.

It should be stated here that, in a normal application (filling calculations), the only component of the F function is liquid metal. In the present model the value F can be composed by liquid metal and by a solid component if the solidification has already started. Consequently F value is at least equal to the value of the solid fraction, this means that if a pct is already solid, only the remaining liquid, “ L ” in eq. (2.18), can be used in feeding shrinkage. A unit value of F corresponds to a full cell; a zero value corresponds to an empty cell.

$$L = (1 - f_s) - \frac{\partial F}{\partial t} \quad (2.18)$$

When the amount of liquid in a cell, “ L ”, reaches zero there is no more liquid metal in this free surface element and the surrounding cells with $F=1$ are activated as free surface continuing feeding the casting enlarging the empty volume. This means that at least one neighbour of a surface cell is a full element, $F=1$, and the feeding velocities are always from inside to outside.

Key point

A 3-D model that is capable of predicting the pressure drop due to shrinkage is presented. The model is based on fluid flow calculation considering a drag force (Darcy term) that is function of fraction solid and on the external surface resistance to move. It considers external defects, in the form of surface depressions, and internal shrinkage defects. By coupling the feed flow, pressure and solidification calculation for predicting shrinkage defects, a complete methodology that enables the possibility to show dynamic shrinkage geometry in the casting and feeding system is presented.

2.3 Boundary conditions

2.3.1. Fluid flow boundary conditions

2.3.1.1. Wall boundary

At solid boundaries the normal velocities are zero, element of case b) in Figure 2.2.

2.3.1.2. Free surface boundary

In free surface boundary elements, element of case a) in Figure 2.2, and elements in Figure 2.3 and Figure 2.4, the continuity equation is not verified. Instead, the F function is calculated to obtain the position of the surface.

The top layer of a casting system, element of case a) in Figure 2.2, is considered to be a free surface element. The pressure of this free surface is set as the atmospheric pressure.

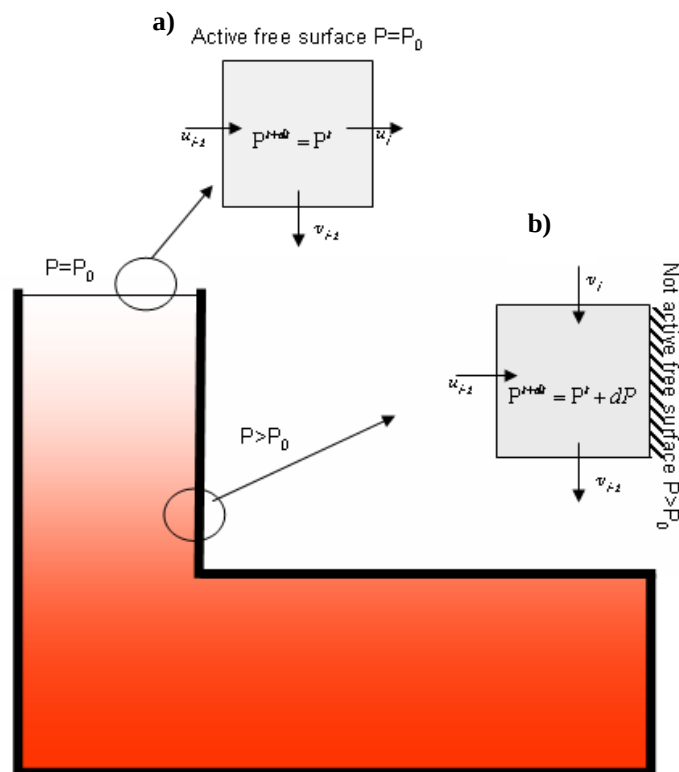


Figure 2.2: Flow boundary conditions a) top free surface boundary b) wall boundary.

During the calculation, the metal at mould interface can also become a free surface if its pressure is lowered to atmospheric pressure and liquid metal can still move (not completely solidified). Thus, the moving interface can partially compensate the material deficit and a surface defect is created (surface depression or a surface connected porosity). Figure 2.3 shows a surface element that has reached the atmospheric pressure and became a free surface element enabling it to feed the casting.

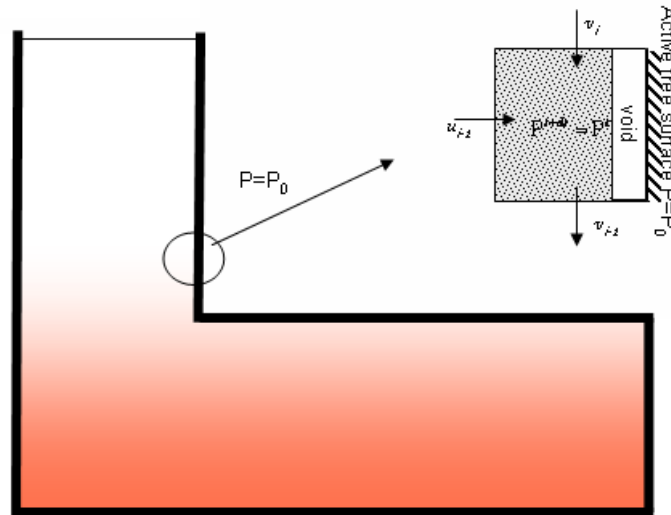


Figure 2.3: Activation of a free surface element.

As the free surface solidifies or the feeding path becomes obstructed, the motion of the free surface stagnates and the pressure quickly drops due to drag force. If a predefined critical pressure is reached, a pore which can act as a feeder will form, Figure 2.4. Once a pore has been opened the pressure in the pore is considered to remain constant.

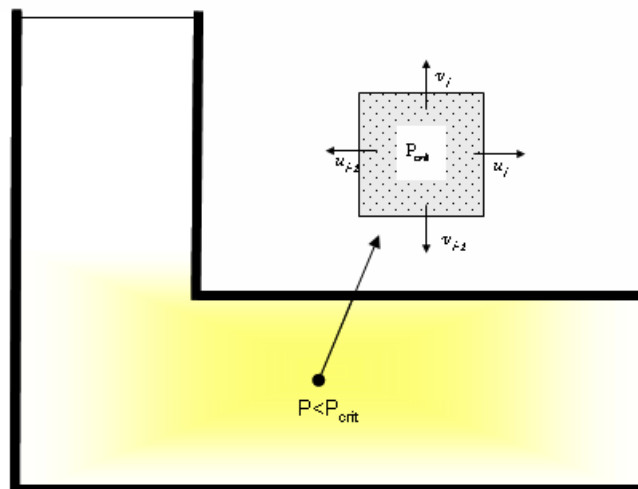


Figure 2.4: Open of a pore.

As a result of these boundary conditions, the only possibility is the liquid going out of a free surface to a full cell.

Key point

Only in free surface elements that have a full neighbour, the term $\frac{\partial F}{\partial t}$ is calculated and it is always negative (inside to outside).

2.3.2. Heat boundary conditions

At the outside of the sand mould, heat is extracted by natural convection only. At the metal and mould interface, a heat transfer coefficient accounts for the thermal resistance at the interface. It is assumed that this heat transfer is not influenced by the movement of the free surface.

2.4 Permeability

In the proposed model (section 2.1) a “drag” term, represented by S , is added to the momentum equation, eq.(2.4), in order to introduce the loss due to resistance of the solidifying material to the feeding flow. In this model the feeding flow is treated as flow through a finely porous media and the Darcy flow, eq.(2.19), is applied as:

$$S = -\frac{\mu}{K} u_i \quad (2.19)$$

where K , represents the permeability and is an important parameter needed in the proposed model. The permeability is related with the solid fraction and solidifying morphology.

2.4.1. Experimental measurements

The first systematic measurement of liquid permeability in the mushy zones of alloys was made by Piwonka and Flemings (1966) who used molten lead to measure the permeability of liquid metal in Al-4.5% Cu alloy. Later, Apelian et al. (1974) measured the permeability of water in partially solidified dendritic networks of aluminium-silicon alloys, and Murakami and Okamoto (1984) used a transparent borneol-paraffin system to study permeability at solid fractions between 0,5 to 0,7 in equiaxed structures.

While the above measurements yield valuable estimates of permeability, the primary disadvantage to these approaches is that the liquid used for the experiment was not the eutectic liquid, and thus the result may not be representative of actual castings [Nasser-Rafi, Deshmukh, and Poirier 1985].

To overcome this problem, many studies used eutectic liquid to measure the permeability in both equiaxed [Streat and Weinberg, 1976; Nasser-Rafi, Deshmukh, and Poirier, 1985; Poirier and Ganesan, 1992; Poirier and Ocansey, 1993; Ocansey, Bhat, Poirier, and Finn, 1994; Paradies, Arnberg, Thevik, and Mo, 1995] and columnar [Poirier, 1987; Nasser-Rafi, 1985; Murakami, 1983-1984] dendritic structures.

Poirier and Ganesan (1992), made measurements on equiaxed structures using aluminium-copper alloys and correlated permeability to the alloy microstructure by the Kozeny-Carman relation:

$$K = \frac{(1 - f_s)^3}{K_c S_v^2} \quad (2.20)$$

where f_s is the solid fraction, S_v is the specific solid surface area, i.e., surface area of solid in unit volume of sample, and K_c is the Kozeny-Carman constant, which takes on various values depending of the characteristics of the porous medium [Carman, 1937].

Ocansey (1994), performed one permeability measurement at a solid fraction of 0.917 using the procedure described in [Poirier, 1992].

A common way of presenting permeability measurements is to plot a dimensionless permeability, $K_s S_v^2$, function of liquid fraction.

Figure 2.5 shows the results from this studies [Poirier, 1992; Ocansey, 1994] plotted in this form, along with the Kozeny–Carman relation.

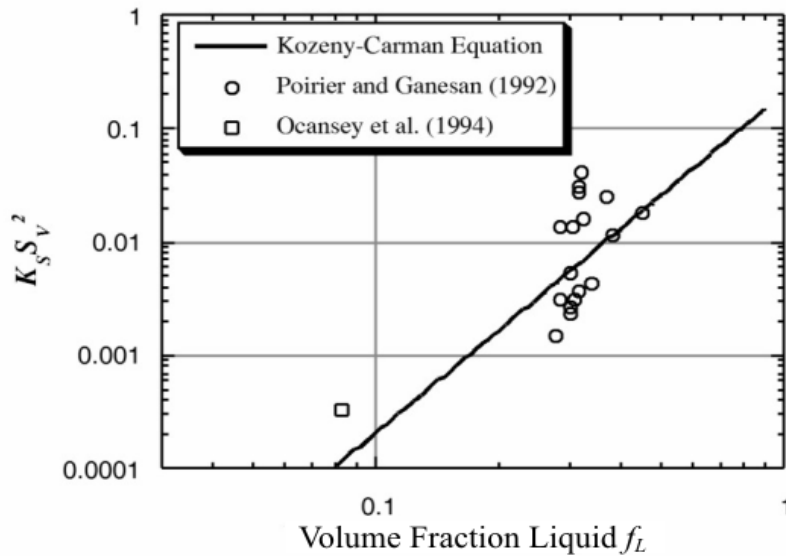


Figure 2.5: The Kozeny- Carman equation ($K_c=5$). Data for aluminium-copper alloy from the literature [Poirier and Ganesan, 1992; Ocansey, 1994] with the Kozeny- Carman equation.

Viswanathan (2001), measured liquid permeability and S_v in aluminium-copper and aluminium-silicon alloys. In this study permeability was also measured using packed glass beads and water, because measurements could be conducted in the absence of

microstructural coarsening. Experimental data was compared with the Kozeny–Carman equation to determine the value of K_C , the Kozeny–Carman constant. The results indicate that when $K_C = 5.0$, all the instantaneous permeability data agree well with the Kozeny–Carman equation. Details of this experience can be found on reference [Viswanathan, 2001].

A comparison between the measured data, the Kozeny–Carman relation and the previous studies [Poirier, 1992] and [Ocansey, 1994], is given in Figure 2.6. The solid line is the Kozeny–Carman equation when $K_C = 5.0$. The solid triangles are data for aluminium-silicon alloys, the solid diamonds represent data for aluminium-copper alloys (Al-8.68 and Al-15.42 % Cu alloys), and the solid circles are data from glass beads.

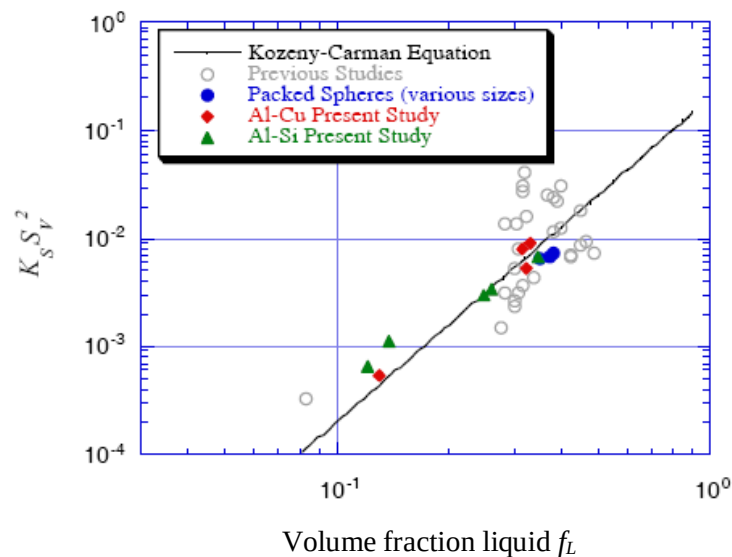


Figure 2.6: Values of dimensionless permeability, and liquid volume fraction, f_L , measured [Crada, 2001] plotted in relation to the Kozeny-Carman equation plotted for $K_C = 5$ and compared to data from literature. [Poirier and Ganesan, 1992; Ocansey, Bhat, Poirier and Finn, 1994].

Key point

Importantly, the results of this study, Figure 2.6, confirm that the Kozeny-Carman equation allows an accurate representation of liquid permeability in the mushy zones of alloys, allowing greater confidence in the use of Darcy's law for calculating pressure distributions during solidification.

2.4.2. Microstructural parameters

The Kozeny-Carmen equation is used to relate the alloy permeability to microstructural parameters [Murakami and Okamoto, 1984; Poirier and Ganesan, 1992; Ocansey et al., 1994]. The S_v parameter in Kozeny-Carmen is dependent on microstructural details, namely, cell spacing: primary and second arm spacing.

In solidification AlSi alloys usually develop a dendritic microstructure [Backerud, 1990]. A dendritic structure is an arrangement of primary, secondary and occasionally higher degree branches, which results in an intricate array in which the spaces between the dendrite arms are occupied by eutectic, Figure 2.7.

The microstructural characterization features are represented in terms of a characteristic dimension that can account for the primary and/or secondary dendrite arms spacing.

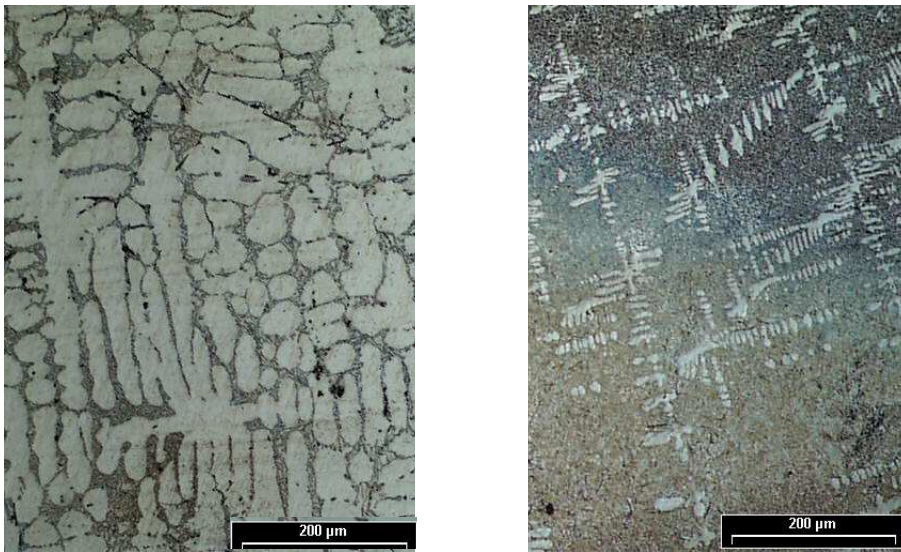


Figure 2.7: A typical microstructure found in AlSi7 and AlSi12 castings (Fluoridric acid etches 8%).

Figure 2.7 shows a typical microstructure found in AlSi7 and AlSi12 alloys castings. Figure 2.8 shows a schematic representation of the microstructural parameters Primary dendrite arm spacing λ_1 and secondary dendrite arm spacing λ_2 .

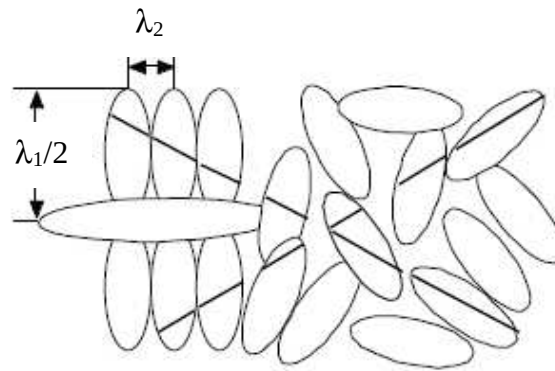


Figure 2.8: Schematic representation showing the characteristic dimension λ_1 and λ_2 .

2.4.2.1. Primary dendrite arm spacing λ_1

a. Data from literature

Figure 2.9 [McCartney, 1981] shows experimental averaging values for λ_1 measured in AlSi castings for several Si concentrations and under the same cooling conditions. Results showed very little dependency on silicon content.

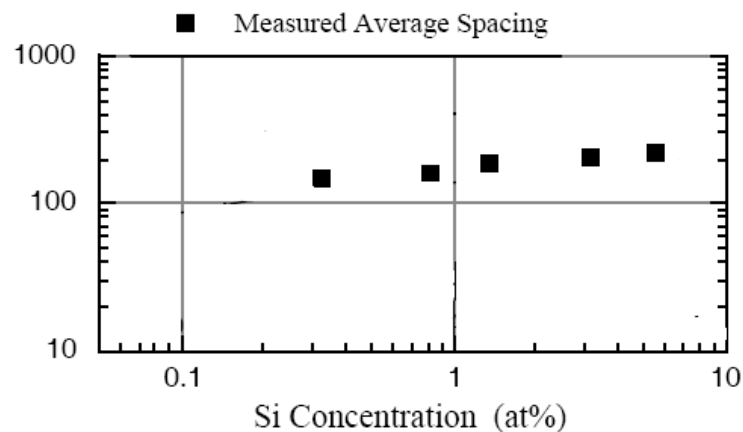


Figure 2.9: Experimental results for primary dendrite arm spacing for AlSi alloys [McCartney, 1981].

Peres (2004) also made experimental measurements of λ_1 for different contents of Si and also from his results he concluded that λ_1 didn't change with Si content.

Figure 2.10 shows experimental measurements made in several AlSi alloys for different cooling conditions, showing the dependence of this parameter on solidification rate. Lower rate gives higher value for λ_1 .

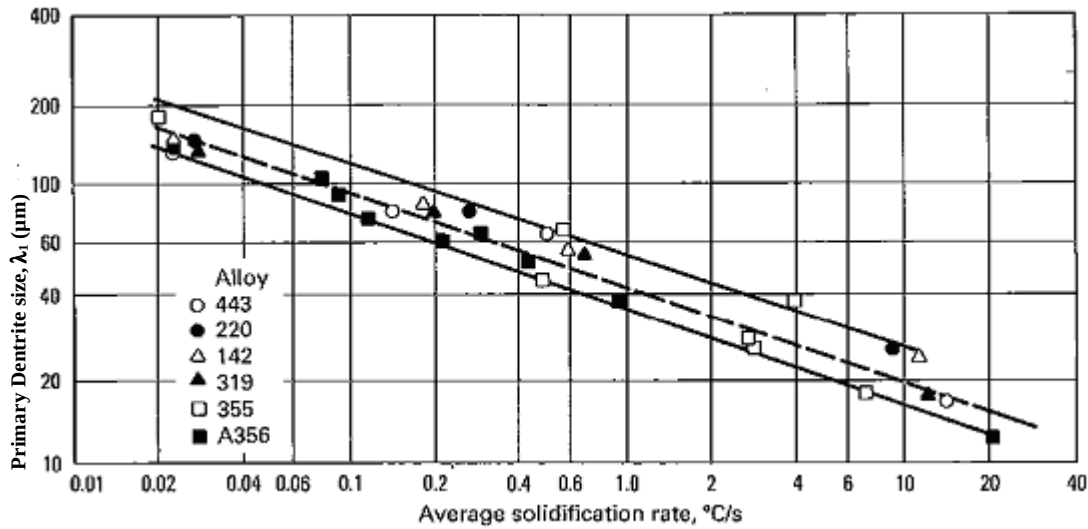


Figure 2.10: Experimental measurements for primary dendrite arm spacing as a function of cooling rate for several aluminium casting alloys [Casting, 1998].

Key point

λ_1 measured in AlSi castings for several Si concentrations and under the same cooling conditions showed very little dependency on silicon content.

b. Analytical Expressions

Numerous solidification models have been developed with a view to characterize dendrite spacing under experimental circumstances [Hunt, 1976; Kurz, 1981; Triverdi, 1984; Hunt, 1996, 1984; Mortesen, 1991; Bouchard, 1997; Chen, 1998; Gundus, 2002].

Hunt's model (1996) can be used to predict primary dendrite spacing under various casting conditions for AlSi alloys. Figure 2.11 shows the calculated primary dendrite spacing at various temperature gradients and growth velocities covering a large range of casting conditions.

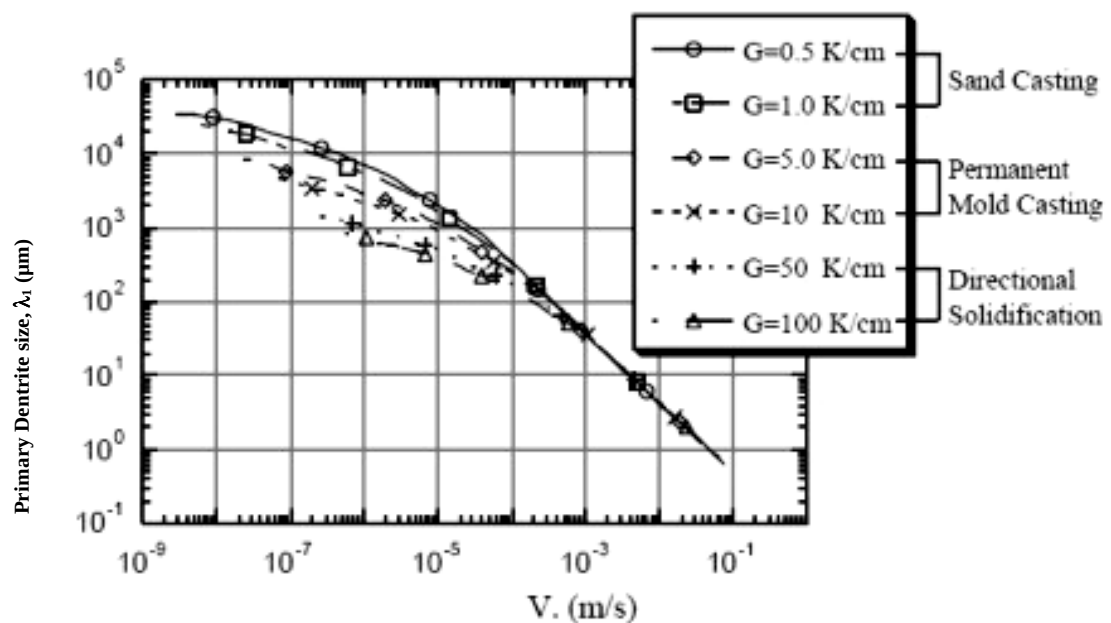


Figure 2.11: Primary arm spacing function of solidification rate for different casting conditions [Viswanathan, 2001].

From Figure 2.11 it is perceptible that for solidification rates above 1E^{-4} , λ_1 is only function of this value and the relation in (2.21) can be used to predict the primary arm spacing [Viswanathan, 2001].

$$\lambda_1 = 0.0576V^{-0.94} \quad (2.21)$$

2.4.2.2. Secondary dendrite arm spacing λ_2

a. Data from literature

In order to evaluate the influence of λ_2 in mechanical properties, Peres (2005) made experimental study, where measurements of λ_2 for AlSi7 for different castings conditions were obtained. The results are shown in Figure 2.12.

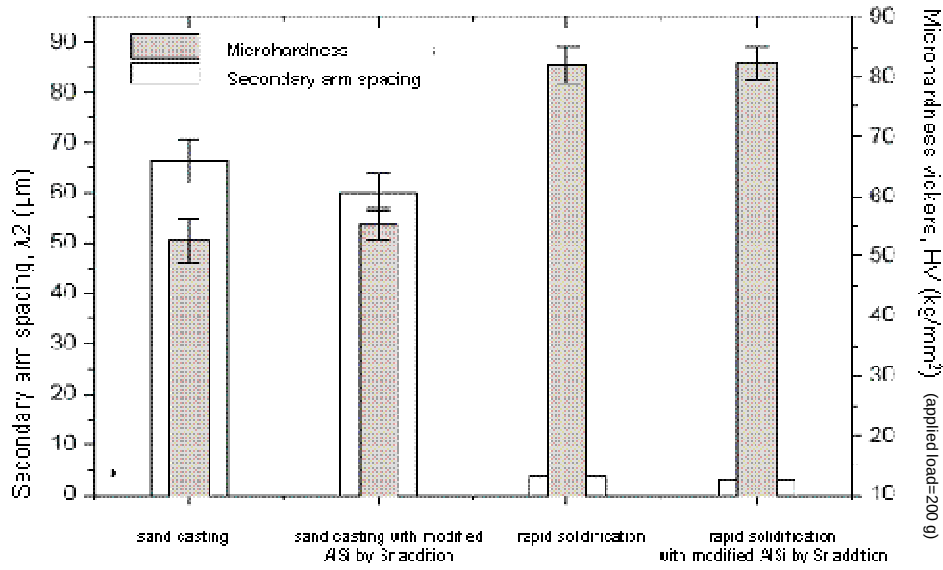


Figure 2.12: Experimental measurements of λ_2 in AlSi7 for different casting conditions [Peres, 2005].

b. Analytical expressions

In literature, several models that are based on experimental data are available. These empirical models reveal that it is convenient to relate experimental results on secondary dendritic arms to the local solidification time.

Bamberger (1987) reported that the secondary dendrite arm spacing during unsteady solidification of hypoeutectic AlSi alloys is related to the local solidification time by:

$$\lambda_2 = B t_f^a \quad (2.22)$$

where “ a ” and “ B ” are dependent on the alloy characteristics.

Bower (1966) proposed the following parameters for (2.22) relationship:

$$\lambda_2 = 7.5 \times 10 E^{-6} (t_f)^{0.39} \quad (2.23)$$

This model was compared with experimental data by Melo (2004) and results suggested that the Bower model described well the variation of secondary arm spacing.

2.4.3. Macrostructure

In terms of macrostructure, castings usually present dendritic solidification that can be equiaxed, Figure 2.13a), or columnar, Figure 2.13b).

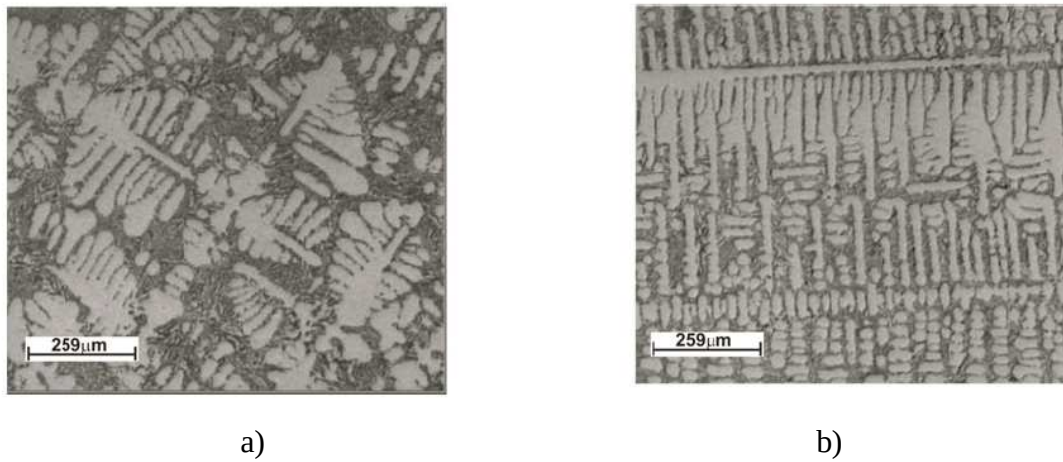


Figure 2.13: Typical dendritic macrostructure found in AlSi casting a) equiaxed and b) columnar.

The Kozeny-Camen relation has been used extensively to model flow through both **columnar dendritic** [Poirier, 1987; Nasser-Rafi, 1985; Murakami, 1983-1984] and **equiaxed dendritic** regions [Poirier, 1985; Poirier and Ganesan, 1992; Poirier and Ocansey, 1993; Ocansey, Bhat, Poirier and Finn, 1994].

For equiaxed solidification, isotropic permeability is commonly accepted. However, it is useful to recall that the Blake–Kozeny expression provides isotropic permeability but due to the directional nature of columnar dendrites, its straightforward application may not be valid (section 2.4.3.2).

2.4.3.1. Equiaxed dendritic

Most solidification models [Chang, 1994; Carlson, 2003] assume the relationship for S_v similar to that for packed beds of spherical particles that is:

$$S_v = \frac{6f_s}{d_c} \quad (2.24)$$

Considering $K_c=5$, eq.(2.20), for permeability, can be rewritten as:

$$K = \frac{d_c^2}{180} \frac{(1-f_s)^3}{f_s^2} \quad (2.25)$$

where d_c is a characteristic dimension, dependent on microstructural details. For simplification the quantity $\frac{dc^2}{180}$ is termed as K_0 and called permeability coefficient and permeability is written as:

$$K = K_0 \frac{(1-f_s)^3}{f_s^2} \quad (2.26)$$

Another approach is to determine S_v from stereological relationships, [Viswanathan, 2001; Sabau, 2002] as:

$$S_v = \frac{4}{d_c} \quad (2.27)$$

$$\text{resulting: } K_0 = \frac{dc^2}{80} \quad (2.28)$$

$$\text{and } K = K_0 (1-f_s)^3 \quad (2.29)$$

The two permeability models, eq. (2.26) and eq.(2.29), are plotted in Figure 2.14 for the same characteristic dimension.

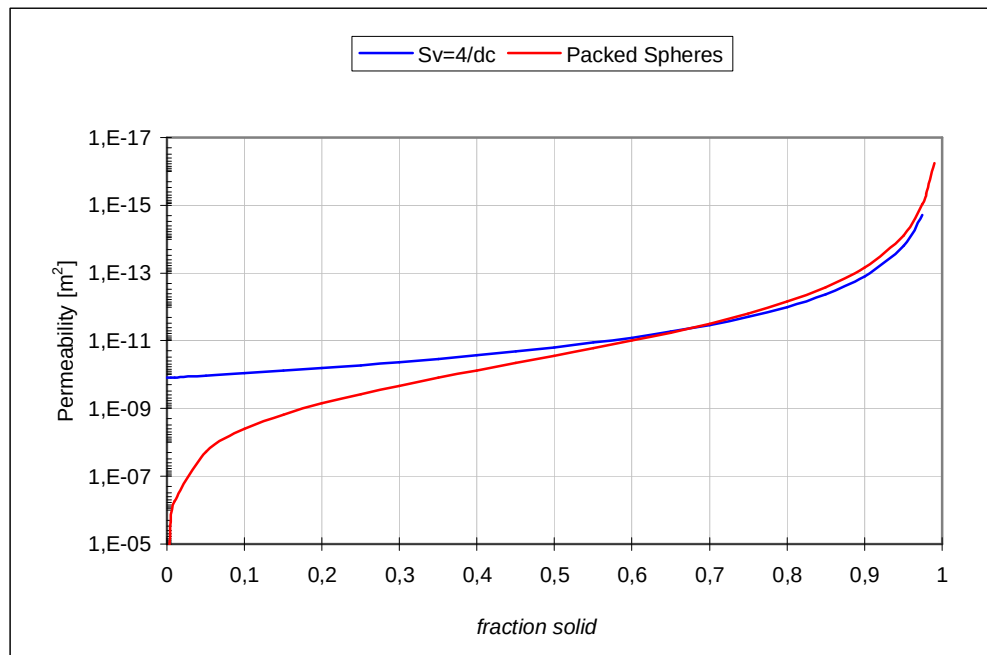


Figure 2.14: Permeability function of fraction solid.

From Figure 2.14, when $S_v=4/d_c$, at solid fractions lower than 0.3, permeability values are unrealistic. Therefore, the relationship $S_v=4/d_c$ is not valid at low solid fractions, i.e., below the coherency point [Backerud, 1990].

The coherency point is considered the value where the mass feeding stops. Below this solid fraction, in early stage of solidification of Al-Si, small equiaxed grains can nucleate and grow in an undercooled melt, Figure 2.15. The solid liquid mixture can be considered as slurry where solid crystals are suspended in viscous melt and can move with the liquid, often referred to as mass feeding. Thus the flow can't be considered interdendritic, and the permeability predicted with eq.(2.26) also can't be used to describe the early stages of dendritic or eutectic solidification. The fraction solid at the coherency point is taken as 0,3 for aluminium alloys [Veldman, 2001].

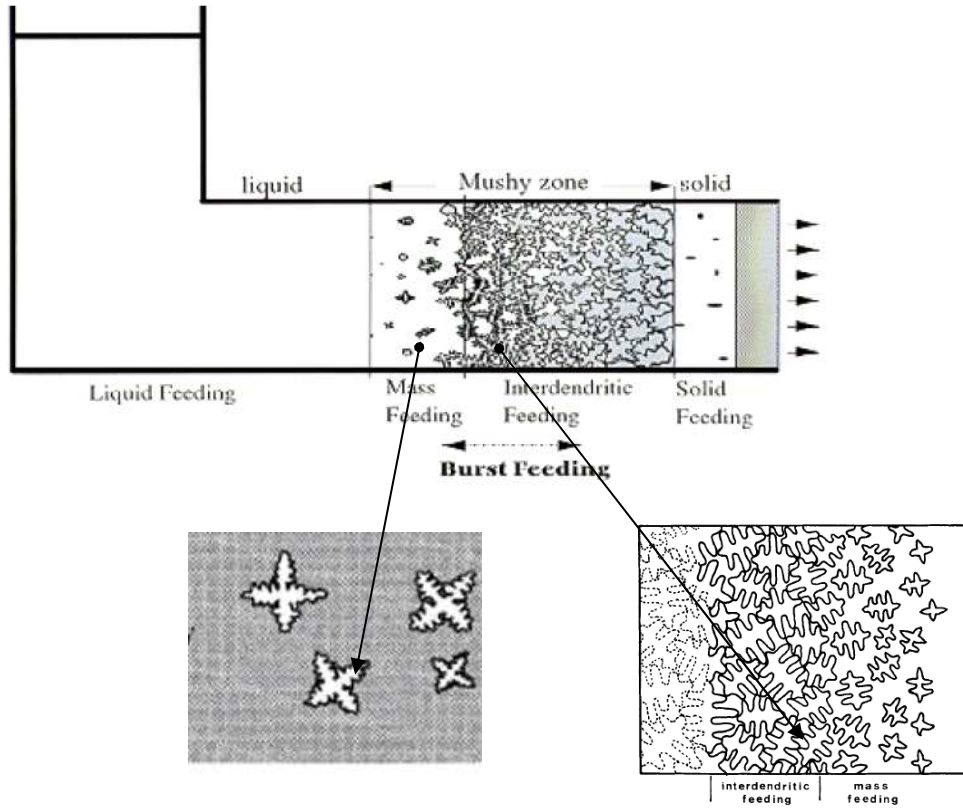


Figure 2.15: Feeding mechanisms. Detail of mass and interdendritic feeding.

In order to use the Kozeny–Carman equation at low solid fractions, Han and Viswanthan (2001) suggested a two step formulation where the dendrite coherency point is taken into account when computing K_s .

$$S_v = \frac{4f_s}{d_c \cdot f_{coeh}} \quad \text{if } f_s < f_{coeh}$$

$$S_v = \frac{4}{d_c} \quad \text{if } f_s > f_{coeh}$$

This model is plotted in Figure 2.16 with and without considering the coherency fraction together the model for packed spheres.

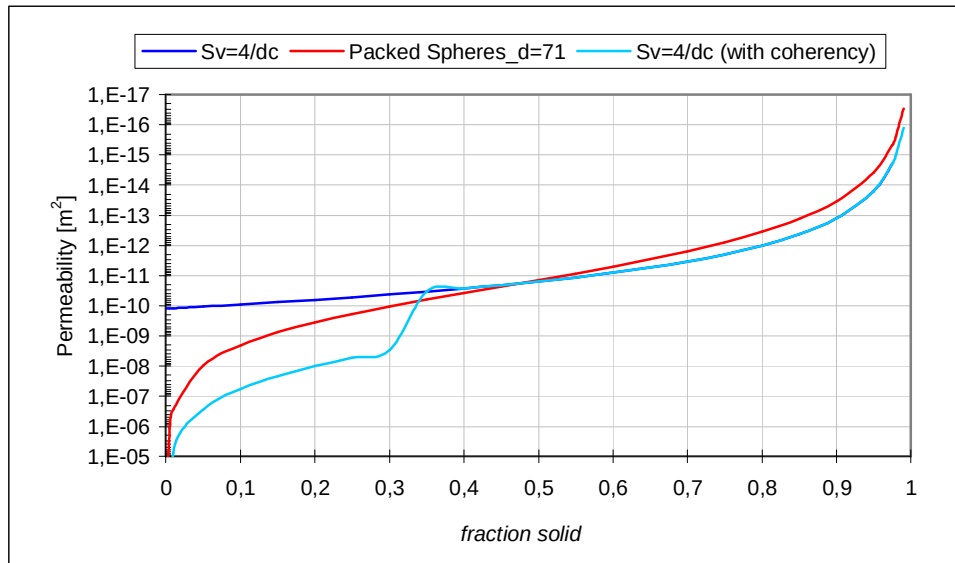


Figure 2.16: Permeability functions of fraction solid.

Another approach to model flow behaviour for fraction solid below 0,3 is to use experimental data to fit a value for K_0 .

Since there are no data directly available from permeability measurements, the data used were from measurements of relative viscosity as a function of fraction solid, for an aluminium alloy determined by Quaak (1996). To derive a value for K_0 the function K is scaled to an equivalent viscosity.

Considering Poiseuille's law that is used to determine the flow rate between two parallel plates as:

$$Q = -w \frac{d^3}{12\mu} \frac{\partial P}{\partial x} \quad (2.30)$$

Where w is the width and d is the height between the two plates (this equation can be derived by the force balance in the control volume similar to that development of Poiseuille):

Combining with Darcy law:

$$\frac{\partial P}{\partial x} = -\frac{\mu_0}{K} v \quad (2.31)$$

it gives a relation between the viscosity and the permeability K :

$$\mu = \frac{d^2 \mu_0}{12K} \quad (2.32)$$

and the relative viscosity given as:

$$\frac{\mu - \mu_0}{\mu_0} = \frac{d^2}{12K} - 1 \approx \frac{d^2}{12K} \quad (2.33)$$

replacing K by the Kozeny-Carmen relation comes:

$$\frac{\mu - \mu_0}{\mu_0} \approx \frac{d^2}{12 K_0} \frac{f_s^2}{(1 - f_s)^3} \quad (2.34)$$

Equation (2.34) relates the relative viscosity, with fraction solid. Using the values determined by Quaak for viscosity as a function of the solid fraction several values of K_0 were considered and plotted together with the experimental values, Figure 2.17. The chosen value for K_0 was $2.8E^{-10}$.

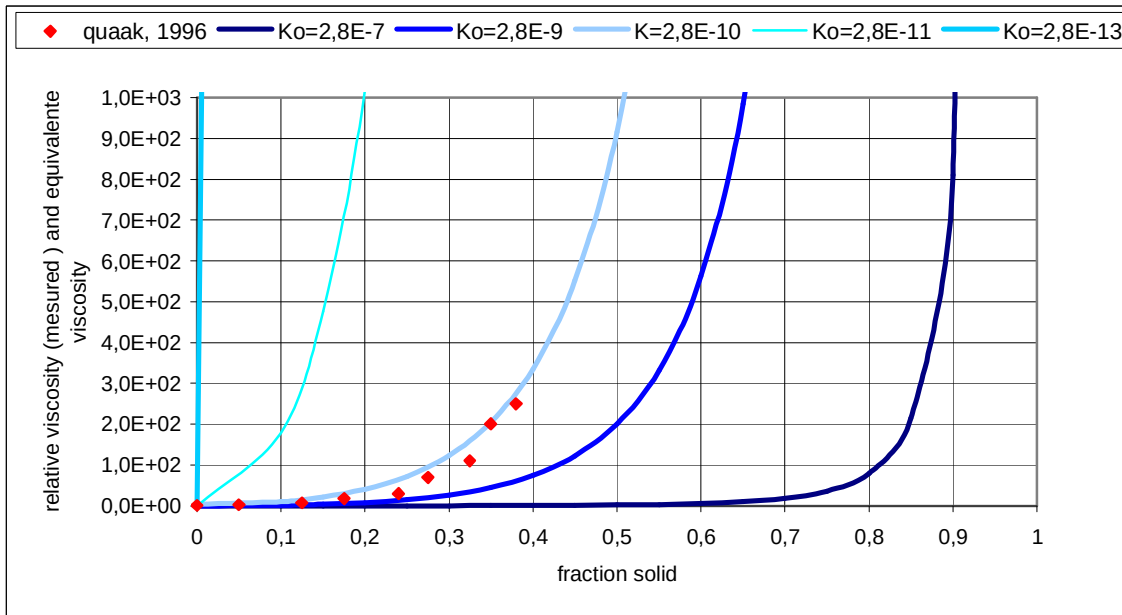


Figure 2.17: Measured viscosity [Quaak, 1996] and the equivalent viscosity due to drag parameter K_0 , as a function of the solid fraction.

For the chosen value of K_0 , $2.8E^{-10}$, permeability is plotted together with previous model in Figure 2.18.

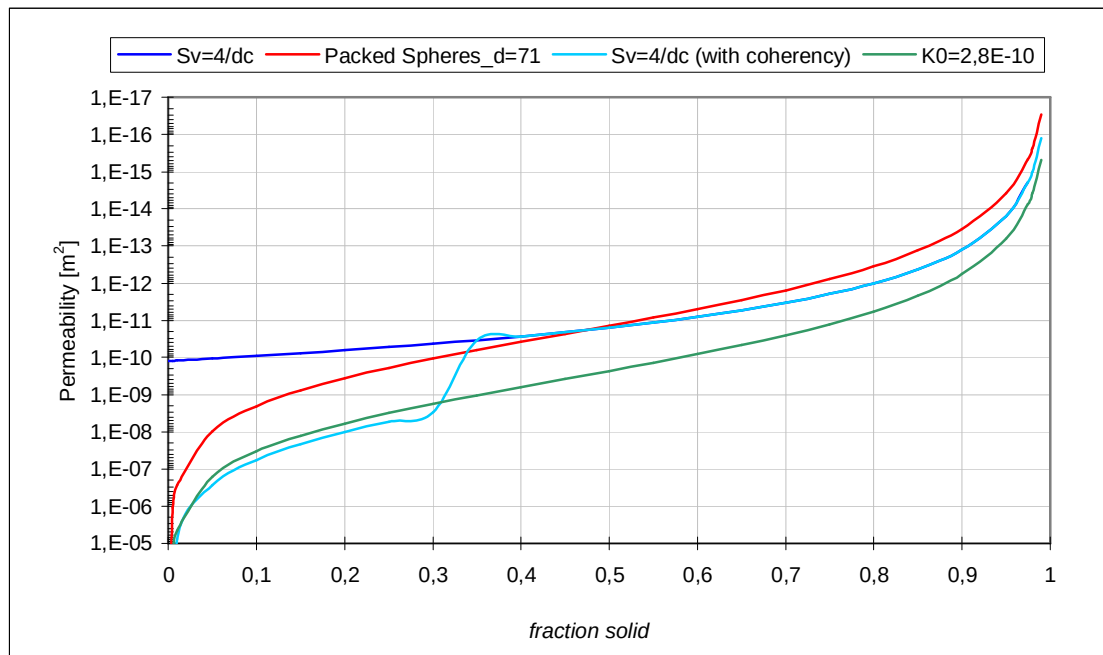


Figure 2.18: Permeability function of fraction solid.

Figure 2.18, shows that the two models suggested for low fractions solids give very comparable results. It's important to notice that this value of K_0 is only valid for fractions solid below 0,3 which correspond to the range of the experimental values used to derive K_0 .

Key Point

A value of $2.8E^{-10}$ is chosen for K_0 , before coherency ($f_s < 0,3$).

After coherency the isotropic permeability coefficient is considered to drops ten times.

2.4.3.2. Columnar dendritic

Due to the directional nature of columnar dendrites, Figure 2.13b), the use of isotropic permeability application may not be valid.

In order to examine the effect of this simplified assumption and the role of the characteristic microstructural dimension, simulation studies were carried out by other authors with both isotropic and anisotropic permeability models with different assumption for the characteristic microstructural dimension schematically presented in Figure 2.19.

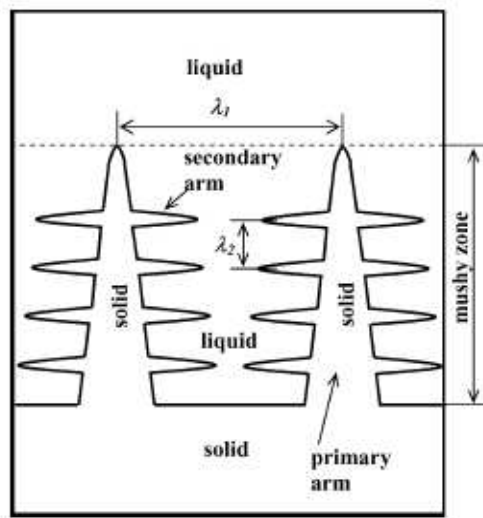


Figure 2.19: Interdendritic channels in a columnar mushy zone showing primary (λ_1) and secondary (λ_2) dendrite arm spacing.

In order to investigate the permeability in columnar solidification Poirier (1987) presented a comparison of various permeability models, in two orthogonal directions, i.e., flow parallel to columnar dendrite, Figure 2.20a), and flow perpendicular to columnar dendrite, Figure 2.20b).

It should be cleared that the purpose of these studies wasn't to model shrinkage defects but, to examine the role of permeability correlation on macrosegregation prediction. Macrosegregation is opposite to microsegregation which is a non homogeneity the scale of a dendrite. Microsegregation is also generated during the solidification of a liquid phase. Macrosegregation is the result of several phenomena including the shrinkage induced feeding flow that depends on the definition of a permeability model. So, the results from this type of studies are also valid for use in our model.

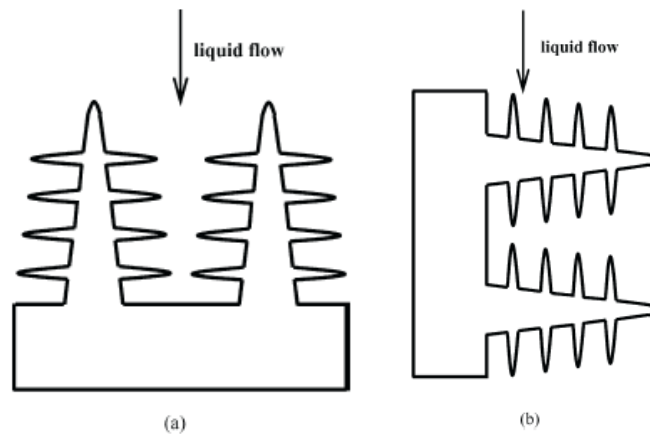


Figure 2.20: Schematic representation of fluid flow parallel (a) and normal (b) to dendrite arms (primary).

Of various models describing flow parallel to dendrites, Poirier (1987) found that the multilinear regression-based model based on experimental data and the Hagen–Poiseuille model gave almost identical results. Since the Hagen–Poiseuille model has a physical basis, this correlation was chosen to describe the flow parallel to the dendrites. The model was tested for solid fraction in the range of 0.39 and 0.83. Beyond this range Poirier recommended the use of Blake–Kozeny model.

For flow perpendicular to the dendrites, Poirier (1987) recommended use of a multilinear regression based model for f_s between 0.34 and 0.81 (permeability data are available within these boundaries only). Beyond this range, the Blake–Kozeny expression was recommended for the permeability value. For the characteristic dimension the authors considered that the dependency on primary arm spacing, i.e., $dc=\lambda_1$.

Recently, Singh (2006), in order to validate his macrosegregation model, presented a comparison, Table 2.1, for different permeability models and permeability coefficient, K_0 . For this purpose, data from the numerical and experimental investigations of [Krane 1997] were used. Macrosegregation profiles at various planes of casting were obtained. Dendrite arm spacing was also measured.

Three case studies were performed, Table 2.1. In case I and II, the Kozeny–Carman isotropic model was used with two different coefficients for permeability. K_0 was related to microstructure through the relationship:

$$K_0 = \frac{d_{c^2}}{180} \quad (35)$$

Table 2.1 – Permeability models and microstructural parameters used in the model.

Case I: Isotropic Blake–Kozeny model for all fs with $K_0 = 1.68 \times 10^{-10} \text{ m}^2$. ($dc=174 \text{ } \mu\text{m}$)

Case II: Isotropic Blake–Kozeny model for all fs with $K_0 = 2.68 \times 10^{-11} \text{ m}^2$. ($dc=70 \text{ } \mu\text{m}$)

Case III: Poirier anisotropic model.

For flow parallel to dendrite arm:

For $fs < 0.39$, Blake–Kozeny, $K_0 = 1.2 \times 10^{-11} \text{ m}^2$,

For $fs > 0.39$ and < 0.83 , Hagen–Poiseuille, $K = 3.75 \times 10^{-12} (1-fs)^2$,

For $fs > 0.83$, Blake–Kozeny, $K_0 = 1.0 \times 10^{-12} \text{ m}^2$.

For flow perpendicular to dendrite arm:

For $fs > 0.66$, Blake–Kozeny, $K_0 = 4.6 \times 10^{-12} \text{ m}^2$,

For $fs > 0.19$ and < 0.66 , multi-linear regression

$$K = 1 \times 10^{-3} fs^{3.32} d^{2.08} = 4.7 \times 10^{-12} fs^{3.32} \text{ m}^2,$$

For $fs < 0.19$, Blake–Kozeny, $K_0 = 1.3 \times 10^{-12} \text{ m}^2$.

($dc=70 \text{ } \mu\text{m}$)

For case I, an experimentally measured value of dendrite arm spacing [Krane, 1997] of $174 \text{ } \mu\text{m}$ was used, which makes $K_0 = 1.8 \times 10^{-10} \text{ m}^2$. The reported spacing, though not mentioned clearly, appears to be primary dendrite arm spacing.

For case II, a measured secondary dendrite arm spacing, $\lambda_2=70$, has been used in the calculation of K_0 .

The case III uses Poirier's anisotropic permeability model considering the characteristics microstructure dimension as $dc=\lambda_2=70$.

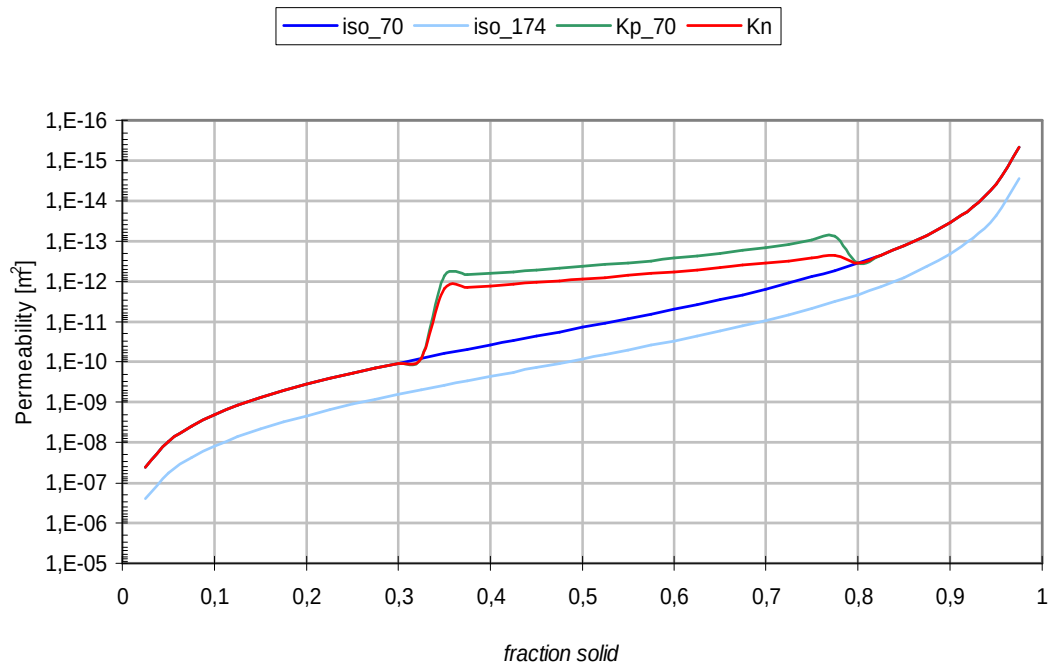


Figure 2.21: Variation with liquid fraction of the perm abilities, perpendicular and parallel to the dendrite arm and the approximate isotropic permeability for two dc.

Figure 2.21 shows K_p , perpendicular permeability, and K_n , normal permeability, as well as the isotropic permeability, as function of solid fraction. The first observation that can be made is that the anisotropic permeability drops by nearly a factor of 100 at the transition point (from slurry to a coherent solid network).

Figure 2.21 also indicates that the permeability parallel to the primary arms is always lower than that perpendicular to the arms, although, the two perm abilities only differ by a factor of around 2 over a large range of liquid fractions.

In Sing (2006) study, these results were compared with the final macrosegregation pattern for all three cases. A good agreement was found for both case II and case III. On the other hand, the Blake–Kozeny model of case I, where permeability coefficient is calculated from $dc=\lambda_1$, results over-prediction of macrosegregation.

Among the three permeability models, case II provided the best match with experimental data. Thus, the secondary dendrite arm spacing seems to control the evolution of macrosegregation for this alloy.

Recently, Santos (2005) proposed a permeability model, eq. (2.36) to eq.(2.38), valid for fs between 0.4 and 0.8 also based on Hagen- Poiseuille law, but considered two characteristic dimension λ_1 and λ_2 , Figure 2.19, by including a tortuosity factor τ .

$$K_n = \frac{(1-fs)^2 \lambda_1 \lambda_2}{8\pi\tau^3} \quad (2.36)$$

$$K_p = \frac{(1-fs)^2 \lambda_1^2}{8\pi\tau^3} \quad (2.37)$$

$$\tau = 1 + \sum_{i=0}^i \left(\frac{\lambda_2}{\lambda_1} \right)^{(1-fs)^i} \quad (2.38)$$

For parallel $i=3$ and for perpendicular $i=2$. This model is plotted in Figure 2.22 together with Sing model and the isotropic model considering the same characteristic dimension, $dc = \lambda_1 = \lambda_2 = 100 \mu m$.

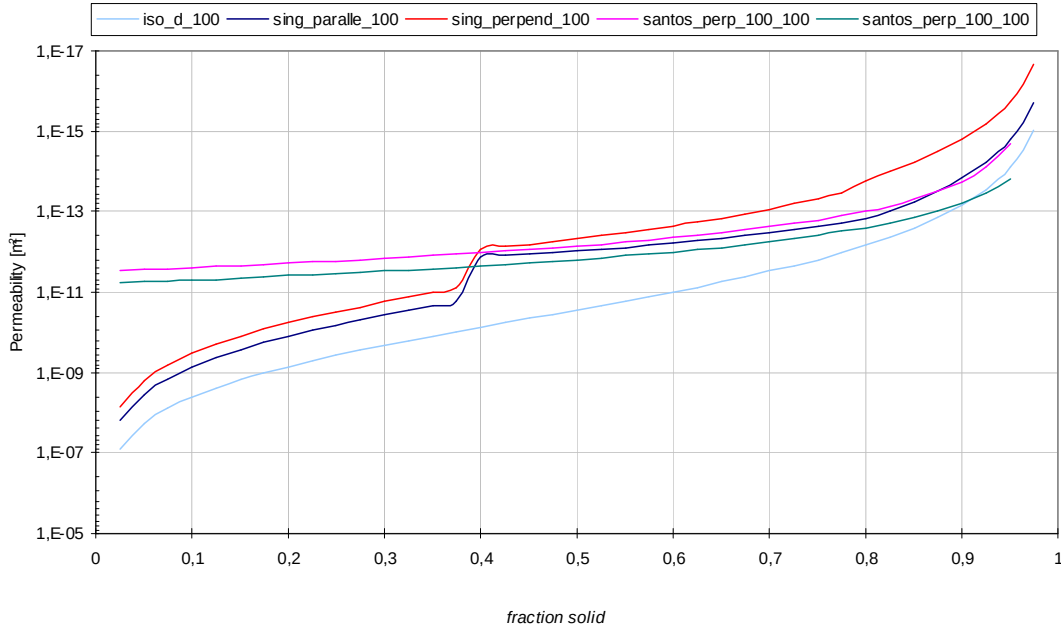


Figure 2.22: Santos model plus Sing model, Figure 2.21, and the isotropic model considering the same characteristic dimension, $dc = \lambda_1 = \lambda_2 = 100 \mu m$.

In order to verify the validity of the relations proposed, results were compared with experimental data obtained by Murakami et al. (1984) and the results obtained showed good agreements. This model, independently of different characteristic dimension considered, also

showed the same evolution with an increase of 100 times in resistance after the coherency fraction was reached.

Key point

If solidification is columnar the permeability coefficient drops 100x in relation to the isotropic coefficient (valid after coherency).

2.4.4. Columnar to equiaxed dendrite solidification

The mass feeding, Figure 2.15, can often be traced to heterogeneous nucleation during the early stages of solidification. Heterogeneous nucleation typically occurs on surfaces of the mould walls, yielding stationary, equiaxed crystals which grow quickly and coalesce or are swept into the melt. Crystals which remain attached experience preferential growth parallel, but opposite to the direction of heat extraction, forming columnar dendrites, Figure 2.23. According with (section 2.4.3.2) when the coherency point is reached for columnar flow the drag force increases 100 times, which outcome an important role to solidification morphologies in feeding flow, specially at wall boundary.

In the free surface after the coherency point is reached the fluidity of the molten metal within the dendrite structure is very restricted, which can be explained based in the fact that in mould interface the solidification is columnar and the permeability in parallel direction is increased one hundred times.



Figure 2.23: Solidification structure found in the mould wall interface.

The transition [Flood, 1998] from an outer columnar to an inner equiaxed grain structure is a common occurrence in metal alloy castings, Figure 2.24, and numerous mechanisms for the columnar-to-equiaxed transition (CET), have been proposed based on experimental evidence.

Gandin (2000b) carried out experiments of the CET in directional solidification of Al-Si alloys with Si contents ranging from 3 to 11 pct and identical thermal conditions. Measured CET positions were similar for all alloy compositions, indicating a weak effect of the Si content.

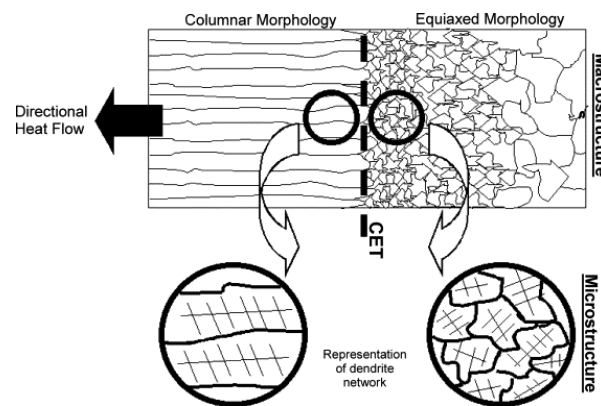


Figure 2.24: Schematic representation of the columnar to equiaxed transition, CET.

Siqueira *et al* (2004) performed CET experiments involving Al-Cu and AlSi alloys by changing the composition, melt superheat, and heat extraction rate at the bottom. They found that a CET criterion based only on either the liquidus isotherm velocity or the temperature gradient ahead of the liquidus isotherm was not supported by their experimental data. Instead, the CET appeared to occur when the cooling rate at the liquidus isotherm decreased below a critical value that was independent of the solute content of the alloy. In this study an average value, 0.20, for the cooling rate at the transition was determined.

Martorano (2003) also measured the CET for different contents of silicon, 3, 5, 7 and 12 pct, and realise that the position of the CET for the same cooling conditions was approximately the same. This can be explained due to compensation, since as the heat transfer coefficient decreases with increase of solute, silicon, the liquidus temperature also decreases.

Compensation between these thermal parameters seems to lead to similar solidification evolution for different contents of Si.

In Figure 2.25 a CET map constructed based on Hunts (1984) model is presented. A CET map draws the transition from the domain columnar to equiaxed.

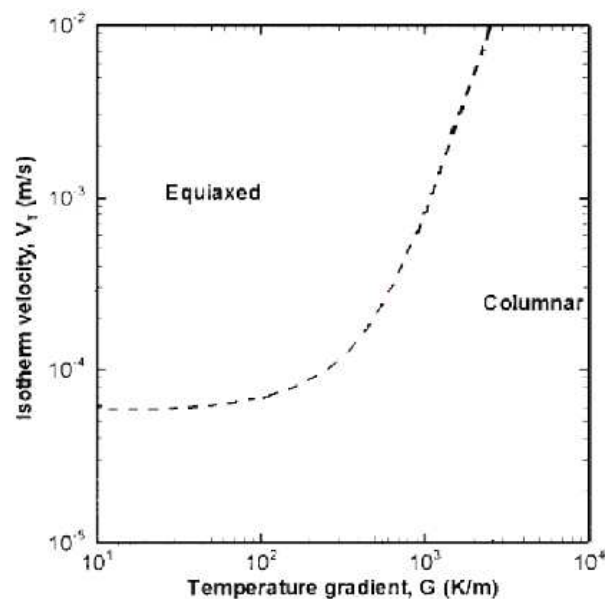


Figure 2.25: CET map for the AlSi7 [Hunt, 1984].

The region below the dashed line represents the range of conditions; isotherm velocity and temperature gradient, which confer a columnar microstructure, opposite, the remaining area of the map will derive an equiaxed structure.

Key point

Si content has very little influence on CET (columnar to equiaxed transition) positions.

2.4.5. Permeability considerations

Since measured primary and secondary dendrite arm spacing were not available, the same are estimated as follows. Experimental and numerical cooling curves, at a few locations in casting (chapter 4), were measured in this work. Using these values, the local solidification time (t_f) solidification velocities (V_s) and the cooling rate C , where estimated, Table 2.2 to Table 2.4 respectively. With these values an average primary and secondary dendrite arm spacing have been estimated.

Table 2.2: Average solidification rate.

Vs solidification rate (m/s)	
AlSi12	$2,7E^{-04}$
AlSi7	$2E^{-04}$

Table 2.3: Solidification time.

t_f (s)	
AlSi12	350
AlSi7	400

Table 2.4: Cooling rate.

C cooling rate (K/s)	
AlSi12	$2,00E^{-02}$
AlSi7	$1,71E^{-02}$

a. Primary dendrite arm spacing

Figure 2.26 show that the model proposed in 2.4.2.1 is suitable to calculate λ_1 , since the solidification rate is in the range of validity of the model (solidification rates higher that $1E^{-5}$).

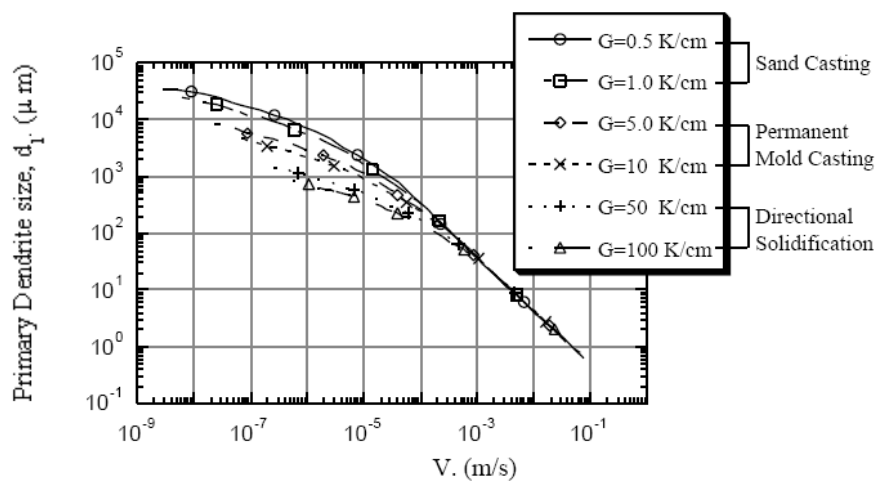


Figure 2.26: Primary arm spacing function of solidification rate for different casting conditions [Viswanathan, 2001].

Table 2.5: λ_1 values.

	$\lambda_1 = 0.0576V^{-0.94} (\mu\text{m})$
AlSi7	154
AlSi12	189

Figure 2.27 show the estimated solidification rate together with experimental values for primary arm spacing found for different AlSi alloys, [Casting, 1998].

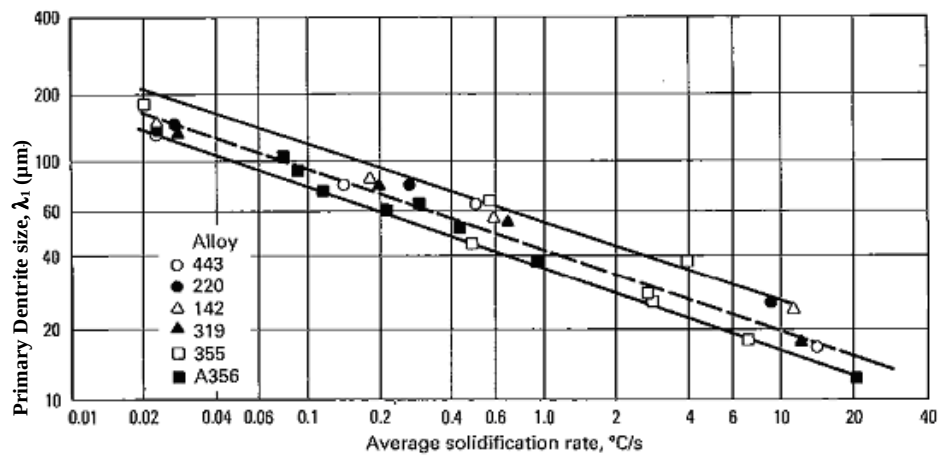


Figure 2.27: λ_1 as a function of solidification rate [Casting, 1998]. The average value found for the solidification rate is superimposed in the graph (red line).

Based on the in these observation, analytical and experimental, and assuming that λ_1 doesn't change relevantly with Si content an verage a value of $170\mu\text{m}$ for λ_1 is adopted.

b. Secondary dendrite arm spacing

The secondary dendrite arm spacing is estimated using the correlation presented in section 2.4.2.

Table 2.6: λ_2 values.

	$\lambda_2 = 7.5(t_f)^{0.39} (\mu\text{m})$
AlSi7	73.6
AlSi12	77.6

Key point

The use of the preceding correlations resulted in secondary dendrite arm spacing in the range of 67 to 75 μm . A mean secondary dendrite arm spacing of 70 μm used in the simulation, which corresponds to $K_0 = 2.8 \times 10^{-11} \text{m}^2$ (valid after coherency and isotropic solidification).

c. Boundary conditions

The permeability will be considered isotropic, except in columnar solidification. Columnar solidification is assumed to occur at surface (mould wall) until a transition distance d_{tran} .

$$\{K_0\} = \begin{Bmatrix} K_0^x \\ K_0^y \\ K_0^z \end{Bmatrix} \text{ and } K_0^x = K_0^y = K_0^z \quad (2.39)$$

The transition distance, d_{tran} , is calculated based on the CET map of AlSi7, Figure 2.28, obtained by Hunt (2000b) (section 2.4.3.2) and compared with critical value of the cooling rate at the liquidus isotherm obtained by Garcia (2005). These values were taken as first approximation in order to use the corresponding permeability model, columnar or equiaxed. Latter this value are tested in chapter 3.

From the cooling curve is possible to calculate the liquidus isotherm velocity as:

$$V_t = \frac{T_{pouring} - T_{Liq}}{t} \quad (2.40)$$

Where $T_{pouring}$ is the pouring temperature and t is the time until liquidus temperature.

Assuming a constant velocity, from the CET map, a value for G (at transition)=500K/m is obtained.

The calculated values are superimposed in CET map for the AlSi7 alloy as shown in Figure 2.25.

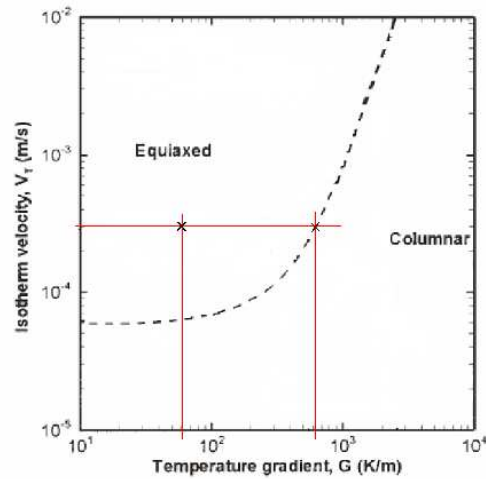


Figure 2.28: Path of solidification plotted in CET map, columnar to equiaxed transition, [Hunt 2000].

From numerical data the temperature gradient was calculated. Considering that:

$$G = \frac{dT}{dx} \quad (2.41)$$

The $G=G_{\text{transition}}$ was found at a distance from surface around $5\text{E}^{-3}\text{m}$.

Also from experimental data, Garcia (2005) found an average transition value for the cooling rate of AlSi alloys. Using this value, $0.17(\text{K/s})$, to calculate the gradient at transition from eq.(2.42):

$$\dot{T} = \frac{G_{\text{transition}}}{V_L} \quad (2.42)$$

A value for $G_{\text{transition}}$ of $550 (\text{K/m})$ was obtained. This value agrees with the obtained in CET map.

As stated in section 2.4.4 the CET distance doesn't vary with the Si content. Therefore, the same distance of 5mm is used for both materials, AlSi7 and AlSi12.

2.4.6. Proposed model

The proposed model has two stages, before and after coherency:

- In the first stage, $f_s < f_{coeh}$, mass feeding will take place and the melt is considered to behave as a slurry. K_0 will take the value found in section 2.4.3.1, $K_0=2.8E^{-10}$;
- in the second stage after coherency, $f_s > f_{coeh}$, the permeability coefficient is set to a 10 times smaller value (decreasing the permeability). The value adopted for K_0 isotropic is $2.8E^{-11}$, which corresponds to using the secondary arm spacing as a characteristic dimension.

For surface elements a special boundary condition that takes into account columnar solidification from surface to the transition to equiaxed, d_{tran} (section 2.4.3.2) is used. In this region permeability is set to 100x lower then the isotropic permeability in the normal direction to free surface, i.e. parallel to surface flow.

Considering $\vec{n}$ as the normal vector to the free surface, $\{1\}$ as the unitary vector and $\{K_0\}$ as the permeability coefficient in the three directions (x,y,z):

$$\{K_0\} = \begin{Bmatrix} K_0^x \\ K_0^y \\ K_0^z \end{Bmatrix} = 2.8E^{-11} \quad (2.43)$$

Key point

Permeability model:

$$\begin{aligned} \{K\} &= 10 \times \{K_0\} \frac{(1-f_s)^3}{f_s^2} && \text{if } f_s < f_{coeh}; \\ \{K\} &= \{K_0\} \frac{(1-f_s)^3}{f_s^2} && \text{if } f_s > f_{coeh} \text{ and equiaxed} \\ \{K\} &= \frac{1}{100} \{K_0\} \vec{n} + \{K_0\} (\{1\} - \vec{n}) \frac{(1-f_s)^3}{f_s^2} && \text{if } f_s > f_{coeh} \text{ and columnar} \end{aligned}$$

All this assumptions are tested in chapter 3.

2.4.6.1. *Simplification in permeability treatment*

Even if the assumptions used to derive permeability are not entirely satisfying, an effective permeability may give usable results when length scale under consideration is sufficiently greater than the microstructural length scale. This macroscale effective permeability depends upon the detailed flow pattern at the microscale, which in turn depends upon the shape and nature of the channels through which the liquid flows. In the dendritic mushy zone, these shapes are quite complex indeed, and both measurement and prediction of the exact flow patterns is difficult.

Another difficulty with the application of the Kozeny-Carman equation lies in the fact that permeability decreases to zero as solid fraction reaches one. In order to limit permeability to non-zero values, it is often considered permeability that is limited by a certain threshold solid fraction. The solid fraction taken as threshold in this work is taken as 0.95.

2.5 Porosity initiation pressure

The pressure in poorly fed regions will drop and if a critical value is reached, P_{crit} , a pore will nucleate. This element is set to a free surface element.

Several values for P_{crit} were considered (tested in chapter 3). In Figure 2.29 some criteria's are presented:

- P1 $P_{crit}=P_{cavitation}$ In general, the cavitation pressures of liquid metals at casting temperatures are very small. At casting temperatures, around 750°C, the cavitation pressure for pure aluminium was determined from published data [Joseph, 2001] to be approximately 10^{-6} atm;
- P2 small pressure drop (0.05atm);
- P3 $P_{crit} = F(fs)$ Several linear functions where the critical pressure is a function of the fraction solid are considered. Although in this work only considers the shrinkage porosity this type of criteria is justified when hydrogen or inclusion contribution is considered. In this case, as the metal solidifies the hydrogen or inclusions are rejected to the liquid and the pressure drop needed to open a pore is lowered.

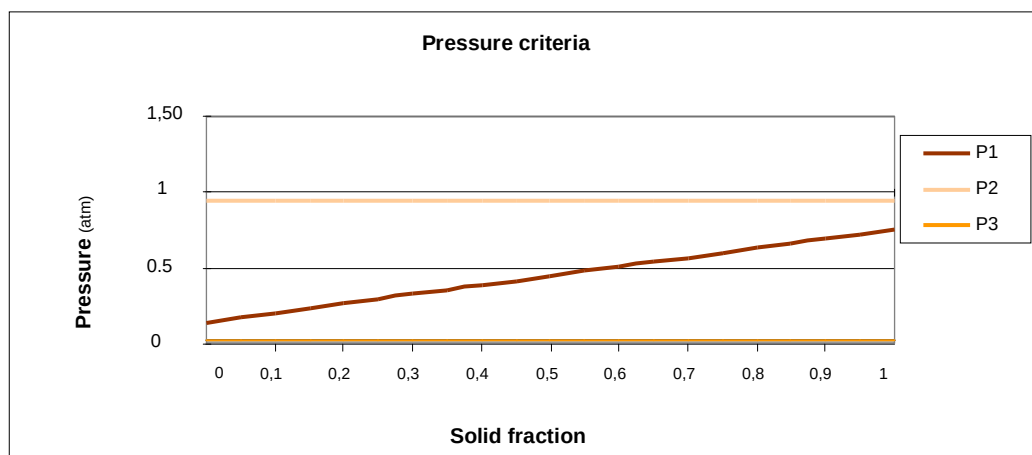


Figure 2.29: Critical pressure criteria.

CHAPTER 3

NUMERICAL MODEL

In this chapter, we shall begin the task of constructing a numerical method for solving the differential equations presented in the previous chapter. This task involves:

- *discretisation;*
- *governing equations;*
- *solution algorithm;*
- *computer model.*

3.1 Discretisation

It is almost impossible to solve the complex differential equations set in chapter 2 analytically in a three dimensional way and therefore a numerical method is used. A numerical solution of a differential equation consists in replacing the continuous information contained in the exact solution with discrete values at a finite number of locations. It is the task of discretisation to establish the position of these nodes by subdividing the geometry into a number of *cells* or *elements*. Since the lines that define the cells and nodes are called *mesh-lines*, the process of discretisation is often called *meshing*.

3.1.1. Spatial discretisation

3.1.1.1. Fixed mesh

For the fixed mesh, the computational cell boundaries are not modified to account for different phase. The liquid continuum equations are extended into the mushy region. This can be seen in Figure 3.1, where there is no distinct interface between the solid, mushy and liquid phase. This method is simple because it lends itself quite easily to the *finite-difference method*.

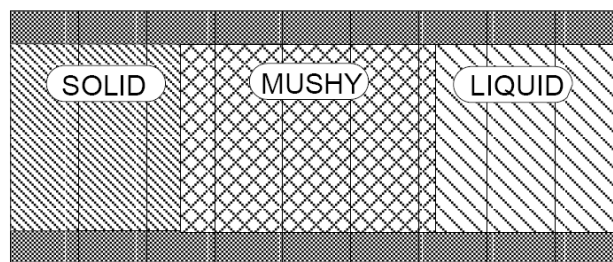


Figure 3.1: Fixed mesh.

3.1.1.2. Non-uniform mesh

Although the mesh may be fixed, it does not need to be uniform. In general, an accurate solution can only be obtained when the mesh is sufficiently fine. There is no need to apply a fine mesh in regions where the dependent variables change slowly with respect to the spatial variable. On the other hand, a fine mesh should be used when the variation is steep. The mesh spacing should be directly linked to the way the dependent variable changes in space.

Notation

At this stage, it is convenient to introduce the notation for spatial discretisation. In Figure 3.2, the x-axis has been subdivided into a number of mesh lines where $\{x_0, \dots, x_i, \dots, x_{ni}\}$, is the position of the i^{th} mesh line and Δx_i is the corresponding mesh spacing. Likewise, the y-axis is subdivided into a number of mesh lines $\{y_0, \dots, y_j, \dots, y_{nj}\}$, where y_j is the position of the j^{th} vertical mesh line and Δy_i the mesh spacing. A node is defined at the intersection of the mesh lines, where ϕ_{ij} can represent the pressure, temperature or velocity of the fluid.

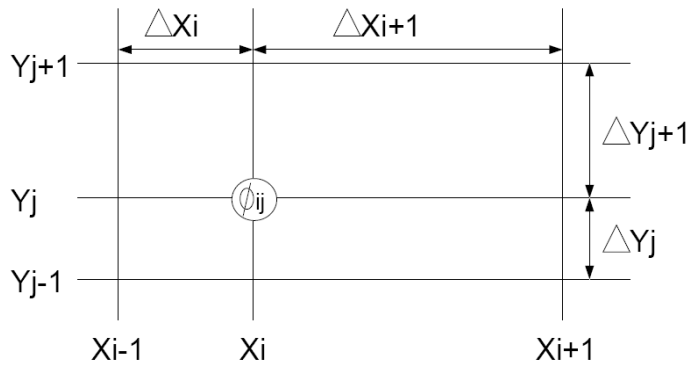


Figure 3.2: non-uniform mesh.

3.1.2. Discrete approximations

The discrete approximation is a set of algebraic relations that connect the independent variables for a group of nodes. Such an equation is derived from the governing differential equation and thus expresses the same physical information.

3.1.2.1. Control-volume approximation

The spatial domain is divided into a number of nodes overlapping control volumes so that there is only one control volume surrounding each node. This is shown as a shaded region in Figure 3.3. The flux into and out of each control volume is calculated across each interface to the control volume.

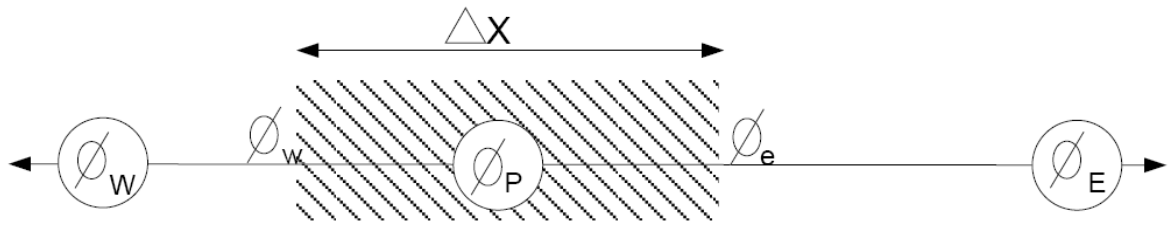


Figure 3.3: One-dimensional control volume.

In this derivation we should apply some assumptions about how the independent variable changes from one node to another.

The central-difference scheme assumes that the convected property at the interface is the average value of the central and adjacent node:

$$\phi_e = (\phi_E + \phi_P)/2; \quad \phi_w = (\phi_W + \phi_P)/2 \quad (3.1)$$

There are two approaches to the creation of a control volume: node-fitted and mesh-fitted. For the moment, since the creation of a control volume is linked to the behaviour of each variable, let us restrict our attention to the temperature variable.

Node-fitted control volume

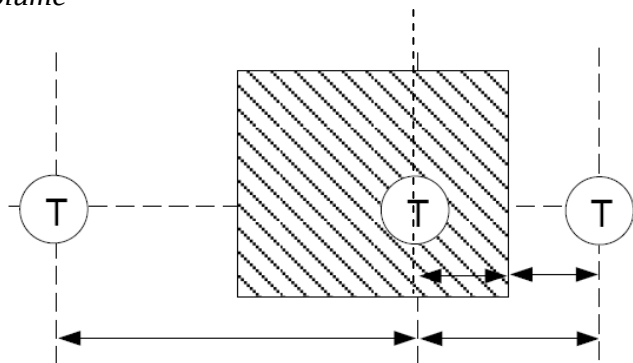


Figure 3.4: Node fitted control volume.

After the geometry is meshed, and the nodes placed at the intersection of mesh lines, a control volume is created around each node, in such a way that the interfaces are located midway between each node. In Figure 3.4, the control volume is shaded and the temperature

nodes are represented by circles. Since the interface is placed equidistant from one node to another, the heat flux across this interface is easy to calculate. This technique suffers from the fact that a temperature node may not lie at the centre of the control volume and thus it cannot be regarded as a good representation of the temperature within the control volume.

Mesh-Fitted Control Volume

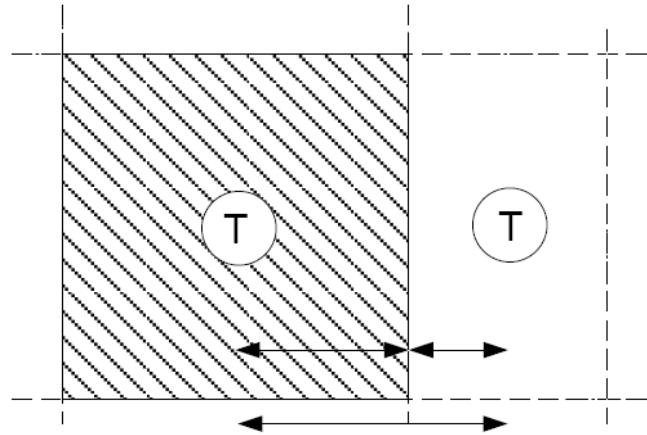


Figure 3.5: Mesh fitted control volume.

Considering the temperature variable, control volumes are first fitted to the mesh and then the nodes are placed at the centre of each control volume. This technique guarantees that the nodal temperature is a good representative of the temperature throughout the control volume, Figure 3.5. It can be seen that control volume turns out to be the basic unit of discretization, but the interface is no longer equidistant from each node. This means that a weighted correction should be applied to the heat flux calculations. Since the effort involved in this calculation is minor, this approach is preferred.

3.1.2.2. Normal mesh

Now that we have chosen the mesh-fitted control volume, we should determine whether it is suitable for the other variables: pressure and velocity. In practice, there appears to be a problem when the pressure and velocity nodes are located at the same point in space. If we examine the momentum equation (chapter 2), the velocity of the fluid is driven by the pressure drop across the control volume. If the velocity and pressure are defined at the same point in space (as in Figure 3.6) then the pressure at the control volume interface should be extrapolated from the surrounding pressure nodes. This means that the central pressure term

will drop out, and the pressure difference will be the difference between alternate nodes. In effect, the pressure is taken from a coarser mesh, one where the momentum equation contains the pressure difference between alternate nodes, not between adjacent ones. Since there is no interaction between adjacent pressure nodes, it is possible to have two independent pressure fields in the same spatial domain. This is unacceptable.

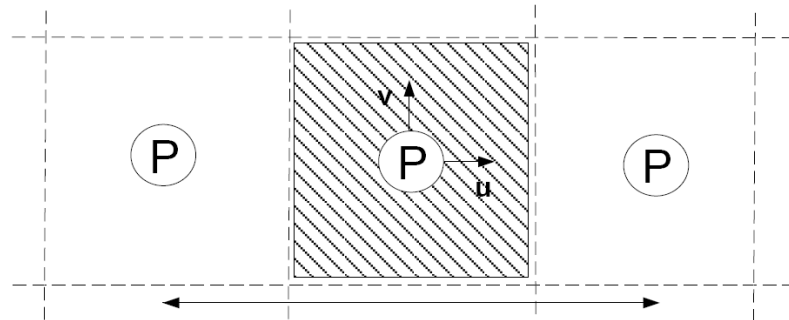


Figure 3.6: Normal mesh.

3.1.2.3. Staggered mesh

There is no reason why we cannot apply a different mesh for each independent variable. In this case, it is convenient to stagger the mesh, so that the velocity of the fluid is shifted to the edge of the control volume. In Figure 3.7, the pressure remains at the centre of the control volume, whilst the horizontal velocity is shifted to the right, and the vertical velocity is shifted upwards. It turns out that this is a more natural way to look at the control volume because the mass flow rates across the control volume interfaces can be calculated without interpolation. The pressure difference between adjacent nodes now becomes the natural driving force for the velocity component located at the interface between each node.

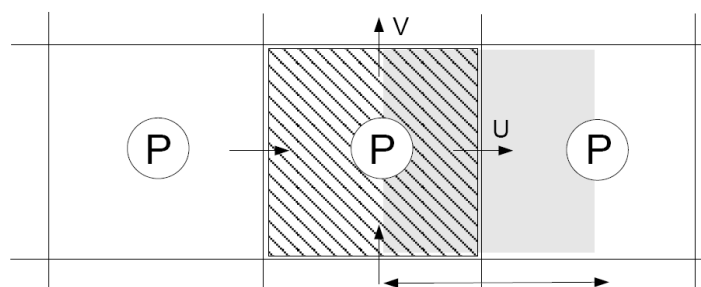


Figure 3.7: Staggered mesh.

While the pressure control volume is still mesh-fitted (stripped in Figure 3.7), the two velocity control volumes are node-fitted (shaded in Figure 3.7).

3.1.3. Temporal discretisation

Since the feeding flow of liquid metal is not a steady state phenomena, it is necessary to discretise the temporal dimension (i.e. the continuous time dimension is subdivided into a set of events $\{t_0, \dots, t_n, \dots, t_f\}$ where t_n is the time of the n^{th} event and Δt_n is the time-step to the next event). The temporal dimension is bounded by the starting, or initial time t_0 , and finishing or final time t_f . At this stage, it is convenient to introduce a new notation ϕ_i^n , where ϕ is a node that can be used for pressure, temperature or velocity, n is the time-step index, and i is the directional index.

Once again, as with the spatial coordinates, the size of the temporal discretisation plays an important role in the accuracy of the final solution. In general, an accurate solution can only be obtained when the time-step is sufficiently small. But then there is no need to have a very small time-step when the dependent variable changes rather slowly with respect to time. On the other hand, a small time-step should be used when the variation is steep. The time-step should be directly linked to the way the dependent variable changes in time.

Now that we have discretised the temporal dimension it is necessary to establish the temporal relationship between one spatial solution and the next. There are two possible extremes:

Explicit: This method assumes that the old data that surround the current node prevail throughout the entire time-step. This means that the $(n+1)$ spatial solution explicitly depends on the previous (n) solution.

$$a_p \phi_p^{n+1} = \sum_i^{nsew} a_i \phi_i^n + b \quad (3.2)$$

Implicit: This method assumes that the new data surrounding the current node prevail throughout the entire time-step. This means that the $(n+1)$ spatial solution is independent of the previous (n) solution and thus should be implicit derived.

$$a_p \phi_p^{n+1} = \sum_i^{n_{sew}} a_i \phi_i^{n+1} + b \quad (3.3)$$

To guarantee stability, the explicit scheme is restricted by a maximum time-step. That is, the time in which it is safe to assume that the surrounding nodes have remained at their old temperatures. This restriction becomes a problem as we reduce the mesh spacing to improve spatial accuracy, because it reduces the maximum time-step. Although the implicit scheme is not restricted in this manner (it is unconditionally stable) if the time step is too large then there is a possibility that it may give an incorrect solution. The choice between the explicit and implicit method will depend on the nature of our problem and the chosen solution algorithm.

3.1.4. Solution to approximation

When the first and second order differential approximations are substituted back into the differential equations from the last chapter we are left with a large number of simultaneous algebraic relationships. To directly solve such a set of equations it would normally require a matrix method. Although there are a number of methods that are very efficient, it's not so easy to overcome the enormous storage requirements that such a problem can present. In fact, in all but the simplest systems, the computer will spend more time swapping data from disk to memory and back, than actually calculating a solution. Fortunately, there is an alternative solution. Since the differential equations are parabolic in time (i.e. one-way) the solution will only depend on the last time-step, and not on any future events. Starting from the initial conditions, the solution can be obtained by marching from one time-step to another. Each solution is a *temporal iteration* of the last. To solve the explicit equation, the new spatial solution for the current time-step is iterated from the spatial solution for the previous time-step. While this is very simple, it is restricted by the stability criterion mentioned in the last section. To avoid this restriction it is necessary to solve the implicit equation. The solution to the implicit equation is complicated by the fact that to calculate the solution for any single node, we need to know in advance the state of all the surrounding nodes. Since the state of the surrounding nodes is not known in advance, an iterative solution should be used (i.e. where the state of the surrounding nodes is estimated, and later improved upon). The iterative solution is started with an initial estimation. The most obvious estimation is to use the solution from the last time-step. After the first iteration, the spatial

solution can be used as the next estimation for the second iteration. This cycle is repeated until convergence, that is, until there is no change to the solution,

$$\max |\phi_p^{m+1} - \phi_p^m| \rightarrow 0 \quad (3.4)$$

where (m) is the $(m)^{\text{th}}$ spatial iteration. The main problem with this technique is that there is no guarantee that any estimation will necessarily be any better than the next. In which case, the iteration may never converge.

The simplest of all spatial iterative methods is the so called *Gauss-Seidel* method, in which the values of the variables are calculated by visiting each node in a certain order. Only one set of data is stored. In the beginning, this data represents the initial estimation or values from the previous iteration. As each node is visited, the variable is updated.

3.1.5. Three dimensions

Although the numerical methods have been explained in a 2 dimensional way, for the sake of simplicity, the model developed is three dimensional. Figure 3.8 and Figure 3.9 present a 3D volume used.

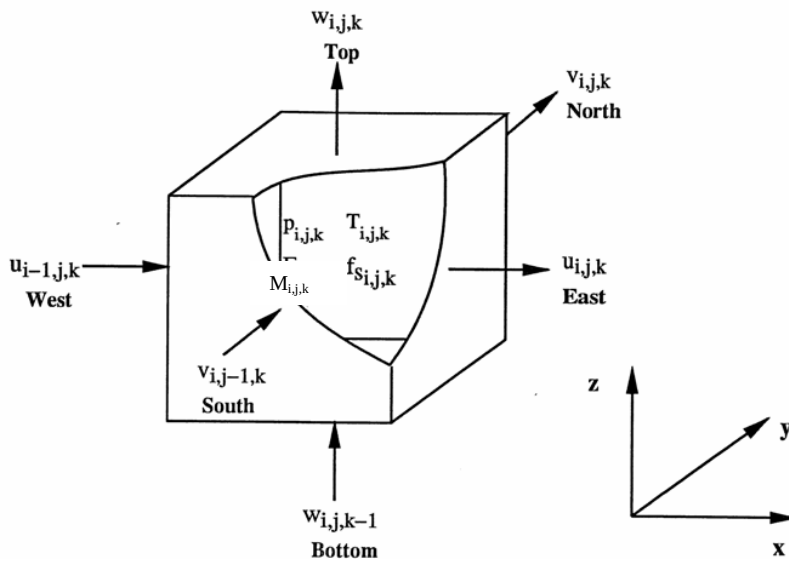


Figure 3.8: Volume element, position of the variables in a staggered grid.

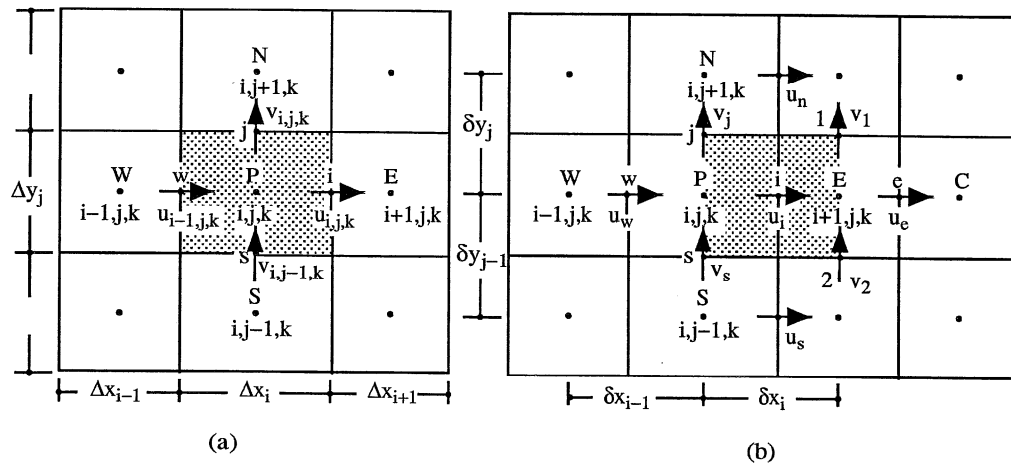


Figure 3.9: Top view of Figure 3.8 a) a main control volume for pressure, temperature etc. b) a control volume for velocity in x direction.

Key point

In this section, we have chosen the following approaches for the current numerical model:

- i. three-dimensional coordinate system;
- ii. fixed, staggered-mesh, finite-difference method;
- iii. mesh-fitted temperature control volume;
- iv. mesh-fitted pressure control volume;
- v. node-fitted velocity control volume;
- vi. explicit and/or implicit solution

3.2 Governing equations

3.2.1. Temperature

In the staggered-mesh formulation, the temperature node lies at the centre of the control volume. This is shown in Figure 3.10 where the control volume is defined by the x and y mesh.

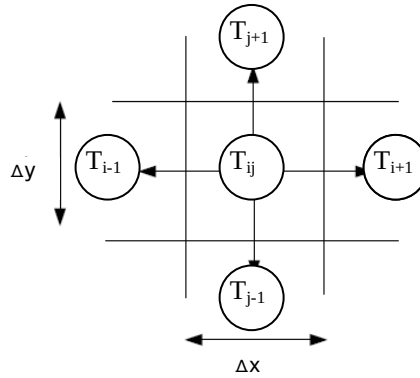


Figure 3.10: Temperature control volume and notation.

Considering the energy equation from chapter 2,

$$\rho C_a \frac{\partial T}{\partial t} + \nabla(\rho C p u_i T) = \nabla(k \nabla T) \quad (3.5)$$

and considering cv as convection term we can write:

$$\rho C_a \frac{\partial T}{\partial t} + cv = k \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) \quad (3.6)$$

with that we can turn into the discretise equation:

$$a_{ij} T_{ij} = a_{i-1} T_{i-1} + a_i T_i + a_{j-1} T_{j-1} + a_j T_j + a_{k-1} T_{k-1} + a_k T_k + a_{ijk}^0 T_{ijk}^0 - a_m conv \quad (3.7)$$

(For simplification one subscript is used; as for example: $u_{ijk} = u_i$; $u_{i+1jk} = u_{i-1jk}$; $u_{i-1jk} = u_{i-1}$) the “0” index indicates a result from a previous time-step.

The coefficients in eq.(3.7) are:

$$\begin{aligned}
a_{i-1} &= k_{i-1} \Delta y \Delta z / dx_{i-1} \\
a_i &= k_i \Delta y \Delta z / dx_i \\
a_{j-1} &= k_{j-1} \Delta x \Delta z / dy_{j-1} \\
a_j &= k_j \Delta x \Delta z / dy_j \\
a_{k-1} &= k_{k-1} \Delta y \Delta x / dz_{k-1} \\
a_k &= k_k \Delta y \Delta x / dz_k \\
a_p^0 &= \rho C_a \Delta x \Delta y \Delta z / dt \\
a_m &= \rho C_p \Delta x \Delta y \Delta z \\
a_{ijk} &= a_{i-1} + a_i + a_{j-1} + a_j + a_{k-1} + a_k + a_{ijk}^0
\end{aligned} \tag{3.8}$$

$$a_{ijk} = a_{i-1} + a_i + a_{j-1} + a_j + a_{k-1} + a_k + a_{ijk}^0 \tag{3.9}$$

And finally the convection term cv comes:

$$\begin{aligned}
cv = & \left[\frac{\Delta t}{2\Delta x_i} \{ (u_{i-1} - 1 + |u_{i-1}|) T_{i-1} - (u_{i+1} - |u_{i+1}|) T_{i+1} + ((u_{i-1} - |u_{i-1}|) - (u_{i+1} + |u_{i+1}|) T_i \right. \\
& + \frac{\Delta t}{2\Delta y_j} \{ (v_{j-1} + |v_{j-1}|) T_{j-1} - (v_{j+1} - |v_{j+1}|) T_{j+1} + ((v_{j-1} - |v_{j-1}|) - (v_{j+1} + |v_{j+1}|) T_j \\
& \left. + \frac{\Delta t}{2\Delta z_k} \{ (w_{k-1} + |w_{k-1}|) T_{k-1} - (w_{k+1} - |w_{k+1}|) T_{k+1} + ((w_{k-1} - |w_{k-1}|) - (w_{k+1} + |w_{k+1}|) T_k \right] \tag{3.10}
\end{aligned}$$

3.2.2. Momentum

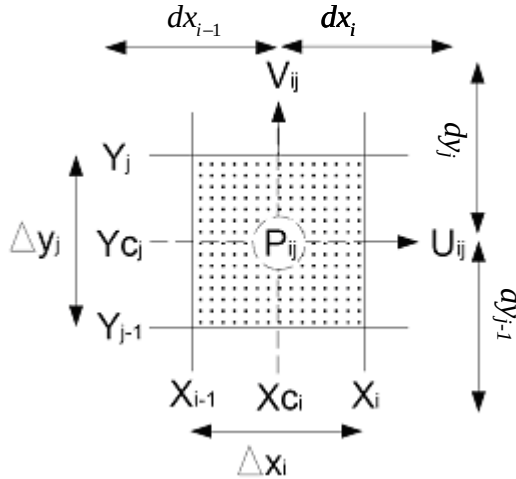


Figure 3.11: Pressure control volume and notation.

Considering a volume as represented in Figure 3.11 the finite-difference approximation of the momentum equations (eq.2.7-2.9) can be written as: (Considering z as the gravity direction, $\rho g_x = \rho g_y = 0$)

$$\begin{aligned}
 u_i \left(\frac{\rho}{\Delta t} + K_x \rho \right) &= \frac{1}{\delta x_i} (P_i - P_{i+1}) + \frac{(\rho u)_i^0}{\Delta t} \\
 u_{i-1} \left(\frac{\rho_{i-1}}{\Delta t} + K_x \rho_{i-1} \right) &= \frac{1}{\delta x_{i-1}} (P_i - P_{i-1}) + \frac{(\rho u)_{i-1}^0}{\Delta t} \\
 v_j \left(\frac{\rho_j}{\Delta t} + K_y \rho_j \right) &= \frac{1}{\delta y_j} (P_j - P_{j+1}) + \frac{(\rho v)_j^0}{\Delta t} \\
 v_{j-1} \left(\frac{\rho_{j-1}}{\Delta t} + K_y \rho_{j-1} \right) &= \frac{1}{\delta z_{j-1}} (P_j - P_{j-1}) + \frac{(\rho v)_{j-1}^0}{\Delta t} \\
 w_k \left(\frac{\rho_k}{\Delta t} + K_x \rho_k \right) &= \frac{1}{\delta z_k} (P_k - P_{k+1}) + \frac{(\rho w)_k^0}{\Delta t} + \rho_k g_k \\
 w_k \left(\frac{\rho_k}{\Delta t} + K_x \rho_k \right) &= \frac{1}{\delta z_k} (P_k - P_{k+1}) + \frac{(\rho w)_k^0}{\Delta t} + \rho_k g_k
 \end{aligned} \tag{3.11}$$

Considering the following simplification:

$$\begin{aligned}
 A_i &= \frac{\rho_i}{\Delta t} + K_x \rho_i & A_j &= \frac{\rho}{\Delta t} + K_y \rho & A_k &= \frac{\rho}{\Delta t} + K_z \rho \\
 A_{pi} &= \frac{1}{\delta x_i} & A_{pj} &= \frac{1}{\delta y_j} & A_{pk} &= \frac{1}{\delta z_k} \\
 B_i &= (K_x \rho u)_i + \frac{(\rho u)_i^0}{\Delta t} & B_j &= (K_y \rho v)_j + \frac{(\rho v)_j^0}{\Delta t} & B_k &= (K_z \rho w)_k + \frac{(\rho w)_k^0}{\Delta t} \\
 A_{i-1} &= \frac{\rho_{i-1}}{\Delta t} + (K_x \rho)_{i-1} & A_{j-1} &= \frac{\rho_{j-1}}{\Delta t} + (K_y \rho)_{j-1} & A_{k-1} &= \frac{\rho_{k-1}}{\Delta t} + (K_z \rho)_{k-1} \\
 A_{pi-1} &= \frac{1}{\delta x_{i-1}} & A_{pj-1} &= \frac{1}{\delta y_{j-1}} & A_{pk-1} &= \frac{1}{\delta z_{k-1}} \\
 B_{i-1} &= (K_x \rho u)_{i-1} + \frac{(\rho u)_{i-1}^0}{\Delta t} & B_{j-1} &= (K_y \rho v)_{j-1} + \frac{(\rho v)_{j-1}^0}{\Delta t} & B_{k-1} &= (K_z \rho w)_{k-1} + \frac{(\rho w)_{k-1}^0}{\Delta t}
 \end{aligned}$$

The resulting discretisation can be written as:

$$\begin{aligned}
 A_i u_i &= A_{pi} (P_i - P_{i+1}) + B_i \\
 A_{i-1} u_{i-1} &= A_{pi-1} (P_{i-1} - P_i) + B_{i-1} \\
 A_j v_j &= A_{pj} (P_j - P_{j+1}) + B_j \\
 A_{j-1} v_{j-1} &= A_{pj-1} (P_{j-1} - P_j) + B_{j-1} \\
 A_k w_k &= A_{pk} (P_k - P_{k+1}) + B_k \\
 A_{k-1} w_{k-1} &= A_{pk-1} (P_{k-1} - P_k) + B_{k-1}
 \end{aligned} \tag{3.12}$$

When the pressure field is given or somehow estimated, these equations can be solved by means of a Gauss –Seidel point-by-point iteration method. But the resulting velocity field will not satisfy the continuity equation, unless the correct pressure field is employed. To solve the discrete equations a solution algorithm is needed. The method used in this thesis is basically the SIMPLE method (Semi-Implicitly Method for Pressure-Linked Equations as developed by Patankar (1980)). In this algorithm, the velocity field based on an estimated pressure field P^* will be denoted by u^* , v^* and w^* which will result from the solution of the following equations:

$$\begin{aligned}
 A_i u_i^* &= A_{pi} (P_i^* - P_{i+1}^*) + B_i \\
 A_{i-1} u_{i-1}^* &= A_{pi-1} (P_{i-1}^* - P_i^*) + B_{i-1} \\
 A_j v_j^* &= A_{pj} (P_j^* - P_{j+1}^*) + B_j \\
 A_{j-1} v_{j-1}^* &= A_{pj-1} (P_{j-1}^* - P_j^*) + B_{j-1} \\
 A_k w_k^* &= A_{pk} (P_k^* - P_{k+1}^*) + B_k \\
 A_{k-1} w_{k-1}^* &= A_{pk-1} (P_{k-1}^* - P_k^*) + B_{k-1}
 \end{aligned} \tag{3.13}$$

And the correct pressure will be obtained from:

$$P = P^* + P' \tag{3.14}$$

For simplicity we now write the equations in the positive direction, where P' is called the correction pressure. The corresponding velocity corrections u' , v' and w' can be introduced in a similar way:

$$\begin{aligned} u &= u^* + u' & v &= v^* + v' & w &= w^* + w' \\ (3.15) \end{aligned}$$

$$\begin{aligned} A_i u_i' &= A_{pi} (P_i' - P_{i+1}') + B_i \\ A_{i-1} u_{i-1}' &= A_{pi-1} (P_{i-1}' - P_i') + B_i \\ A_j v_j' &= A_{pj} (P_j' - P_{j+1}') + B_j \\ A_{j-1} v_{j-1}' &= A_{pj-1} (P_{j-1}' - P_j') + B_{j-1} \\ A_k w_k' &= A_{pk} (P_k' - P_{k+1}') + B_k \\ A_{k-1} w_{k-1}' &= A_{pk-1} (P_{k-1}' - P_k') + B_{k-1} \end{aligned} \quad (3.16)$$

Simplifying:

$$\begin{aligned} u_i' &= \frac{A_{pi}}{A_i} (P_i' - P_{i+1}') = D_i (P_i' - P_{i+1}') \\ u_{i-1}' &= \frac{A_{pi-1}}{A_{i-1}} (P_{i-1}' - P_i') = D_{i-1} (P_{i-1}' - P_i') \\ v_j' &= \frac{A_{pj}}{A_j} (P_j' - P_{j+1}') = D_j (P_j' - P_{j+1}') \\ v_{j-1}' &= \frac{A_{pj-1}}{A_{j-1}} (P_{j-1}' - P_j') = D_{j-1} (P_{j-1}' - P_j') \\ w_k' &= \frac{A_{pk}}{A_k} (P_k' - P_{k+1}') = D_k (P_k' - P_{k+1}') \\ w_{k-1}' &= \frac{A_{pk-1}}{A_{k-1}} (P_{k-1}' - P_k') = D_{k-1} (P_{k-1}' - P_k') \end{aligned} \quad (3.17)$$

Equations (3.17) are called the velocity correction formula. The starred velocities, u^* , v^* and w^* , are corrected in response to the pressure correction:

$$\begin{aligned} u_i &= u_i^* + D_i (P_i' - P_{i+1}') \\ u_{i-1} &= u_{i-1}^* + D_{i-1} (P_{i-1}' - P_i') \\ v_j &= v_j^* + D_j (P_j' - P_{j+1}') \\ v_{j-1} &= v_{j-1}^* + D_{j-1} (P_{j-1}' - P_j') \end{aligned} \quad (3.18)$$

$$w_k = w_k^* + D_k (P'_k - P'_{k+1})$$

$$w_{k-1} = w_{k-1}^* + D_{k-1} (P'_{k-1} - P'_k)$$

3.2.3. Pressure correction equation

Now the continuity equation should be satisfied. The integral of eq.2.2 becomes:

$$\frac{(\rho_{i,j,k} - \rho_{i,j,k}^0) \Delta x \Delta y \Delta z}{\Delta t} + [(\rho \cdot u)_i - (\rho \cdot u)_{i-1}] \Delta y \Delta z + [(\rho \cdot v)_j - (\rho \cdot v)_{j-1}] \Delta x \Delta z + [(\rho \cdot w)_k - (\rho \cdot w)_{k-1}] \Delta x \Delta y = 0 \quad (3.19)$$

Substituting all the velocity components given in equations (3.18) we obtain the following discretisation for the pressure correction equation P' :

$$A_0 P' = (A_1 P'_{i+1} + A_2 P'_{i-1} + A_3 P'_{j+1} + A_4 P'_{j-1} + A_5 P'_{k+1} + A_6 P'_{k-1} + \frac{(\rho^{\text{old}} - \rho^{\text{new}}) \Delta x \Delta y \Delta z}{\Delta t} - D) \quad (3.20)$$

where D is:

$$D = (\rho u_{i,j,k}^* - \rho u_{i-1,j,k}^*) \Delta y \Delta z + (\rho v_{i,j,k}^* + \rho v_{i,j-1,k}^*) \Delta x \Delta z + (\rho w_{i,j,k}^* + \rho w_{i,j,k-1}^*) \Delta x \Delta y \quad (3.21)$$

and

$$A_1 = \rho_i D_i \Delta y \Delta z$$

$$A_2 = \rho_{i-1} D_{i-1} \Delta y \Delta z$$

$$A_3 = \rho_j D_j \Delta x \Delta z$$

$$A_4 = \rho_{j-1} D_{j-1} \Delta x \Delta z \quad (3.22)$$

$$A_5 = \rho_k D_k \Delta y \Delta x$$

$$A_6 = \rho_{k-1} D_{k-1} \Delta y \Delta x$$

$$A_0 = A_1 + A_2 + A_3 + A_4 + A_5 + A_6 \quad (3.23)$$

“ D ” is the divergence which is calculated from the tentative velocity field, this means that if the difference in expression (3.24) comes to zero the continuity equation is satisfied. Thus this difference should be lower than a defined error ε :

$$\left| \frac{(\rho_{i,j,k}^{\text{old}} - \rho_{i,j,k}^{\text{new}}) \Delta x \Delta y \Delta z}{\Delta t} - D \right| < \varepsilon \quad (3.24)$$

3.2.4. Function F

The function F , section 2.2 (free surface treatment), which accounts for the volume of metal in an element, also should satisfy the continuity equation, eq.(2.17). Considering the set of boundary conditions, Figure 3.12, and for one-dimensional, F can be discretised as:

$$F_i^{n+1} = F_i \left[-\frac{\Delta t}{2\Delta x} (u_{i-1} + |u_{i-1}|) - (u_i - |u_i|) + (u_{i+1} - |u_{i+1}|) - (u_i + |u_i|) \right] \quad (3.25)$$

A donor-acceptor method is used. This method is based upon the identification of a cell that is able to donate fluid and another which is able to accept it. The flux between the donor and acceptor cells is calculated from the velocity of the fluid (in filling application the “shape” of the interface between the two cells must also be known).

A free surface can only be enlarged (can't be filled again) and no fluid can come in. Therefore all velocities at a boundary of a free surface cell can only be from the free surface cell to a full cell. The only possible boundary configurations are presented in, Figure 3.12, for one dimensional case:

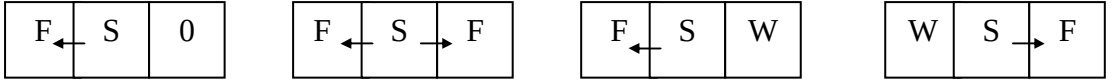


Figure 3.12: One dimensional free surface possible configuration.

where “0” stands for an empty cell, “F” for a full cell, “S” for a free surface cell and “W” for a wall cell. At the interface between a surface cell and a cell that contains fluid, it is reasonable to use the momentum equations to calculate the velocity of fluid at the interface. This is not the case at the interface between a surface cell and an empty cell or a surface cell and a wall, because the velocity at such an interface has no physical meaning. In these cases the velocity is set to “0”. For the situation in Figure 3.13 the function “F” is calculated as:

$$F_i^{n+1} = F_i \left[-\frac{\Delta t}{\Delta x} u_i \right] \quad (3.26)$$

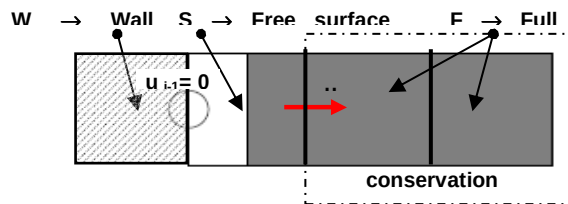


Figure 3.13: Example of function “F” calculation.

3.3 Solution algorithms

The task of this section is to develop a solution algorithm which can solve the governing equations. There are three equations to solve: continuity, momentum and energy. The energy equation can be solved independently because it can be uncoupled from the other two. That is, the solution to the continuity and momentum equation can be used as the starting point to the energy equation. The remaining two equations: continuity and momentum should be solved simultaneously.

3.3.1. Iterative method

An iterative solution is based on the fact that it is only possible to substitute the correct pressure field substituted into the momentum equations when the resulting velocity field satisfies the continuity equation. Since there is no explicit equation that defines pressure in terms of velocity, then the pressure should be estimated. If the continuity equation is not satisfied, then the pressure should be made. If the pressure field is constantly being improved, the velocity field will progressively get closer to satisfy the continuity equation. At some point we should decide to accept the pressure field as being correct. This algorithm is shown in Figure 3.14.

The iterative method relies on being able to correct the pressure, and more importantly that each correction improves with each iteration. A measure of this success is how well it satisfies the continuity eq.(3.27), where the *residual-error* equals:

$$R = (\nabla v) \quad (3.27)$$

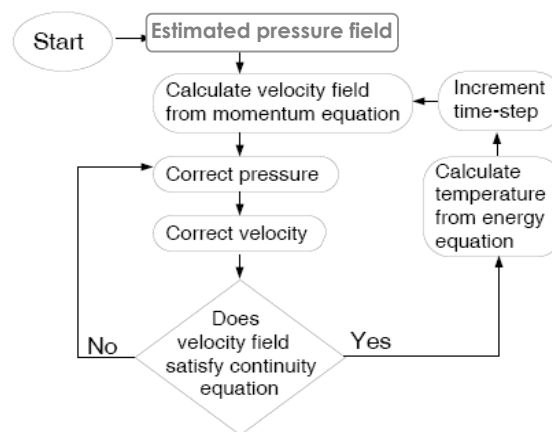


Figure 3.14: Iterative pressure correction algorithm.

The behaviour of the iteration is shown in Figure 3.15. When the *maximum residual error* falls below a predefined limit, the solution is said to have “converged” and the iteration can be stopped. If the slope of the maximum residual-error is positive, the solution is said to “diverge” and the iteration should be aborted.

To allow the solution to stabilize, these tests are only performed after a minimum number of iterations (*min_iterations*). To achieve a convergence within a practical time frame, it is also necessary to define an upper limit to the number of iterations (*max_iterations*). If the solution has failed to converge before it reaches this upper limit, the pressure iteration should be repeated with a smaller time-step. Figure 3.15 shows the relation maximum residual-error versus number of iterations.

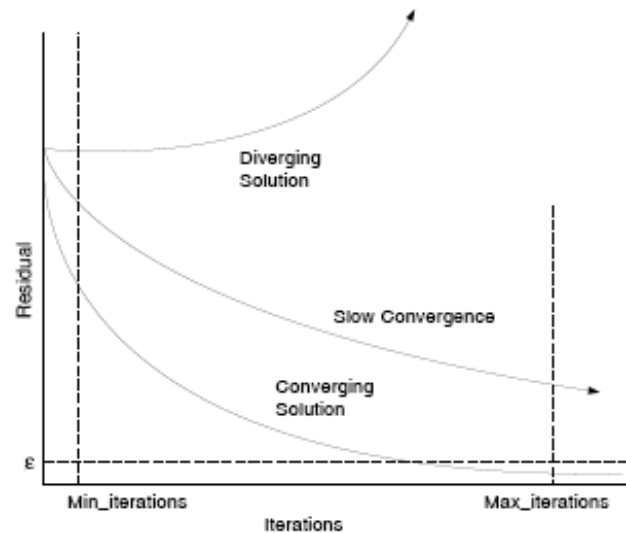


Figure 3.15: Maximum residual-error versus number of iterations.

To solve this coupled equation the “simple algorithm” presented next [Patankar] was used. The SIMPLE method (Semi-Implicit Method for Pressure-Linked Equations) is based on a pressure correction that is defined from the surrounding pressure corrections and the old velocities. If the continuity equation is substituted back into the momentum equation, an expression for the pressure correction is determined.

The basic solution algorithm is the following:

- i. Start with an estimated pressure field P^* .
- ii. Solve the momentum equations to obtain: u^* , v^* and w^* .
- iii. Solve the pressure correction equation P' .
- iv. Calculate $P = P^* + P'$.
- v. Calculate velocities, u , v and w from their starred values using the velocity correction formulas.
- vi. Treat the corrected pressure P as a new estimated pressure, return to step ii and repeat until a converged solution.

Key point

The SIMPLE method (Semi-Implicit Method for Pressure-Linked Equations), is used to solve the coupled pressure velocity equations.

3.4 Computer model

3.4.1. Data structure

3.4.1.1. Geometric data

The geometrical data defines the spatial domain in which the calculations are performed. In the finite-difference method the spatial domain is subdivided by a mesh, Table 3.1.

Table 3.1: Mesh.

Δx	Width of the cell
Δy	Height of the cell
Δz	Length of the cell
dx	distance in x direction across two adjacent cell
dy	distance in y direction across two adjacent cell
dz	distance in z direction across two adjacent cell

3.4.1.2. Thermo physical data

Each material properties of each cell are identified with a property matrix, Table 3.2.

Table 3.2: material properties.

[ρ]	Density
[k]	Conductivity
[cp]	specific heat
[T]	Temperature
[K_0]	Permeability coefficient

The physical state of each cell is represented with matrix, Table 3.3. These matrices should be initiated at the beginning of the calculations.

Table 3.3: Calculated data.

[P]	Pressure
[u]	x velocity component
[v]	y velocity component
[w]	w velocity component
[FS]	Solid fraction
[K]	permeability
[F]	Volume of metal

3.4.1.3. Initial temperatures

Table 3.4: Temperatures.

Tsol	Solid temperature
Tliq	Liquidus temperature
Tamb	Room temperature
Tpouring	Pouring temperature

3.4.1.4. Control data

The control output data are used to terminate the program and to signal it when output data should be written. The iteration control data are used to control the numerical stability and efficiency of the program Table 3.5.

Table 3.5: Control data.

Control output	Stop_average fst	An average value of fs is set to stop calculations
	Write to file	Loop and mode to write data to a file
Control numerical stability	maxerr	Maximum residual error
	iterat_num	Maximum number of pressure iterations

3.4.1.5. Time setup

Since an explicit method is used, the maximum time step is limited. The choice of the time-step is critical to the efficiency of the computer program. If the time-step is too conservative, the program becomes inefficient. If it is too large, the program may become unstable. These opposing criteria lead to an optimal time-step. The following restriction should be made to prevent the fluid flow from more than one cell, in one time-step:

$$dt < \min\left(\frac{dx_i}{u}, \frac{dy_j}{v}, \frac{dz_k}{w}\right) \quad (3.28)$$

The following restriction should be made to prevent the diffusion of heat across more than one cell, in one time-step:

$$dt < \min[dx_i, dy_j, dz_k] \left(\frac{Cp}{8k}\right) \quad (3.29)$$

3.4.2. Boundary conditions

There are two types of boundary conditions: thermal and fluid. The thermal boundary conditions are automatically satisfied with a heat transfer coefficient between each type of material. (The only boundary condition that needs to be imposed is the temperature of the incoming fluid, if convection is considered). The fluid boundary conditions, on the other hand, need to be defined at the following interfaces: wall boundary and free surface boundary.

The [m] matrix stores the “type” of each element. In this matrix, [m], the type of element is identified by an index for each state, defined in Table 3.6

Table 3.6: Metal and boundary identification, matrix [m] index.

1	meta1	Metal element
2	mould	wall element
3	Internal porosity	Internal free surface cell (internal porosity)
4	External porosity	External free surface cell (or free surface connected)
5	Surface	Surface cell
6	empty	Stop feeding (no more liquid available)

Surface boundary (interface mould metal)

By setting to different index we find a way to prevent outflow, if any metal element, [m]=1, has a neighbour index “2” then a surface boundary exists and flow in this interface is set to zero.

Free surface

A free surface element is an element that meets any of the criteria for becoming a free surface element. In this element no conservation law is applied, and therefore melt can flow from the element to feed the casting $0 < F < 1$. If the element has a neighbour that isn’t metal then this element is considered to possess a free external surface and a surface sink or a surface connected porosity will take place. On the other hand if the element is surrounded by metal, an internal free surface is created, initiating an internal porosity.

Heat transfer

The energy boundary condition at this interface is defined by the heat transfer coefficient between the molten metal and the mould material. In the interface between the mould and the surrounding air an heat transfer coefficient is determined from the sum of the convection and radiation losses.

Symmetry

This boundary corresponds to a line of symmetry that exists in the casting configuration. At such a boundary there is no heat or fluid flow across the interface. Whenever possible this boundary condition is used because it halves the number of mesh elements, and thus reduces the storage requirements.

CHAPTER 4

MODEL TESTING AND VALIDATION

The aim of this chapter is to perfectly document the features of the model developed here, by performing a number of theoretical simulations that exhibit well known features of shrinkage related defects and perform sensitivity analysis.

4.1 Predicting internal and surface connected porosity

It is widely recognized that different types of alloy can exhibit quite different forms of porosities in terms of size, type and location. The model described previously (chapter 2) predicts the extent of macroporosity, its location, and type (ie. internal or surface connected). However, there are no validation experiments the author is aware of that are suitable to validate this model with regard to the factor that determines whether shrinkage porosity is occurring either internal or surface connected or both.

To illustrate the features of the model developed, a simple geometry has been simulated. This geometry is a block (35 x 35 x 35mm) surrounded with moulding sand (wall thickness 15mm), Figure 4.1. Two alloys with a binary eutectic phase, a short freezing (small interval between T_{liq} and T_{sol}) and a long freezing alloy (large interval between T_{liq} and T_{sol}), were analyzed. Liquid metal initially at a temperature of 590°C is cooled by a room temperature of 20°C. Table 1 shows the calculation parameters for the two alloys.

Table 4.1: Calculation properties and parameters for short and long freezing alloys.

Properties and parameters	Short freezing	Long freezing
Liquid density (kg/m ³)	$\rho_l = 2600$ (kg/m ³)	$\rho_l = 2600$ (kg/m ³)
Solid density (kg/m ³)	$\rho_s = 2700$ (kg/m ³)	$\rho_s = 2700$ (kg/m ³)
Liquidus Temperature	$T_{liq} = 570$ (°C)	$T_{liq} = 610$ (°C)
Solidus Temperature	$T_{sol} = 565$ (°C)	$T_{sol} = 565$ (°C)
Initial melt Temperature	$T_0 = 590$ (°C)	$T_0 = 590$ (°C)
Conductivity	$= 181$ W(m.K)	$= 181$ W(m.K)
Heat capacity	$= 1150$ (W/(kg.K))	$= 1150$ (W/(kg.K))
Cdrg (permeability constant)	10E4	10E4

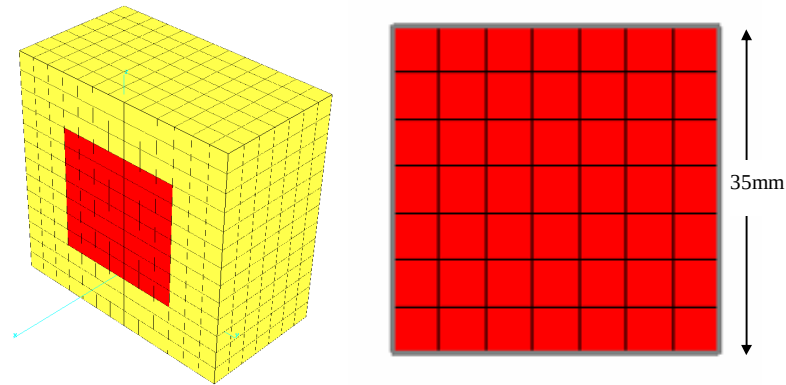


Figure 4.1: Mesh, metal plus sand for cup test.

4.1.1. Short freezing material

As the metal material solidifies, the liquid fraction needs to compensate for the mass deficit. Initially unrestrained feeding occurs and the liquid metal level will sink uniformly over the complete top surface. Because the edges of the cube solidify first and form the first dendrites, the surface sinks most in the middle resulting in a sloped top surface, Figure 4.2. As the solidification progresses, high fractions solid appear in the outer layers of the cube.

The pressure and solid fraction distribution are shown in Figure 4.4 for at 68 % solidification. At this instance the indicated cell meets the criterion $P < P_{crit}$. A free surface is created and the pore will grow as it takes over the feeding from the sinking outside, Figure 4.4 and Figure 4.5. It should be noted that the formation of the pore has immediately influence on the flow velocities, which change direction from inwards to outwards.

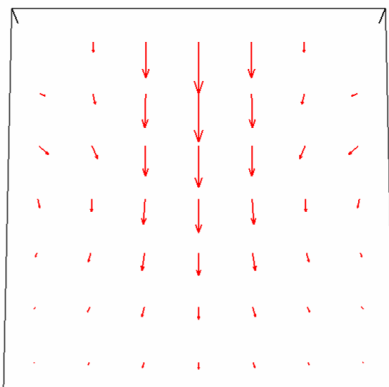


Figure 4.2: Feeding velocity field, short freezing alloy 68% solid ($v_{max} = 7 \cdot 10^{-5} \text{ m/s}$).

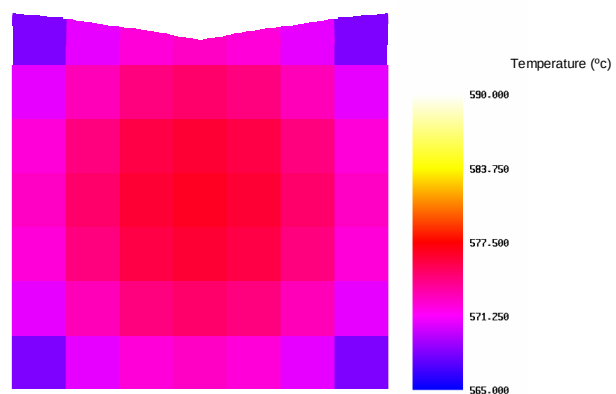


Figure 4.3: Temperature distribution represented with the contour of the free surface (external).

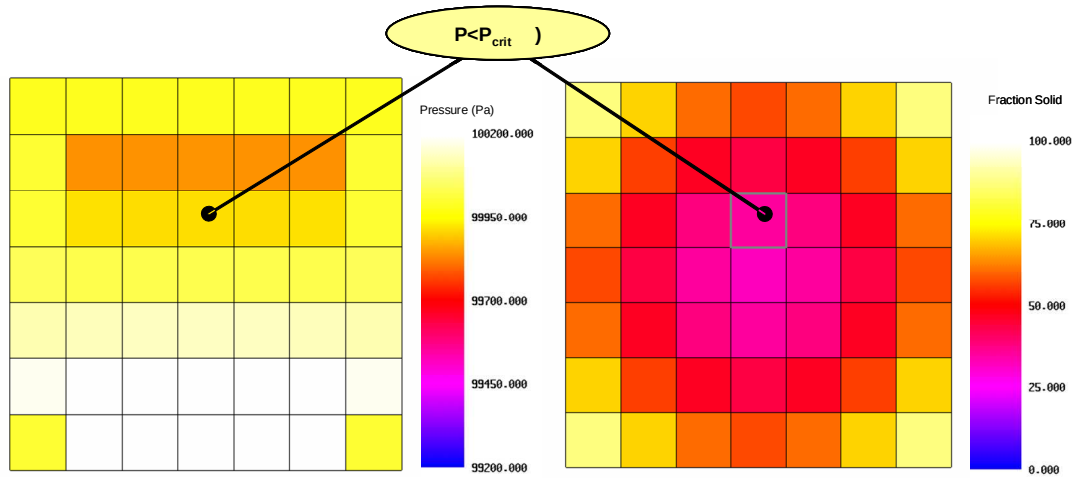


Figure 4.4: Pressure and fraction solid distribution, short freezing alloy (68% solid).

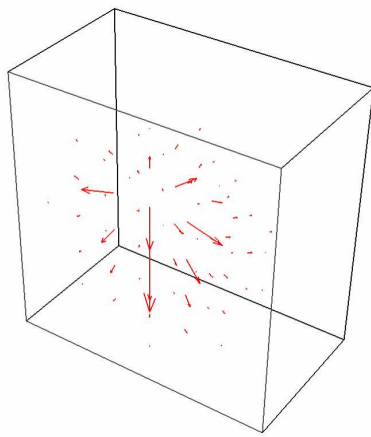


Figure 4.5: Velocity field, short freezing alloy 68% solid ($v_{max} = 15. (10E^{-5} \text{ m/s})$).

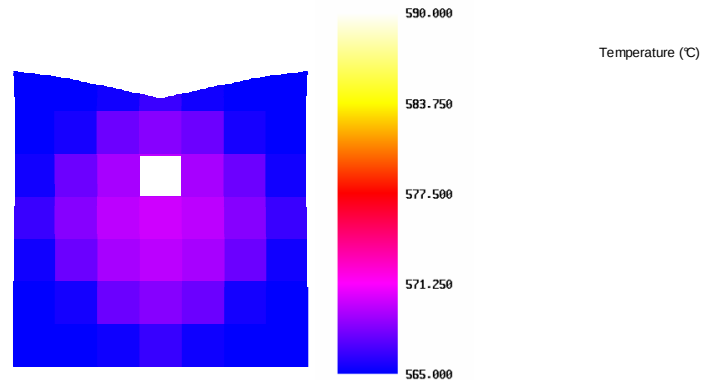


Figure 4.6: Temperature distribution represented with the free surface contour (internal).

4.1.2. Long freezing material

In the long freezing material the top feeding velocity is much more uniform, Figure 4.7, resulting in a flatter top surface, Figure 4.8. Until an average solid fraction of 90 % the pressure to open a pore is not reached. Thus all the shrinkage is compensated by the outside layer. Figure 4.7 shows clearly that the velocities go from out to inside resulting in sinking of the outer surface, Figure 4.8.

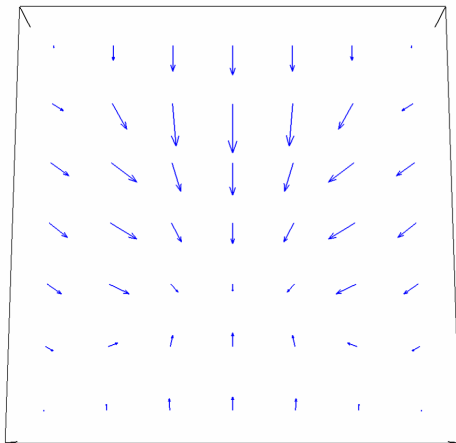


Figure 4.7: Velocity field for long freezing, 90% solid ($v_{\max} = 0.5 \times 10^{-5} \text{ m/s}$).

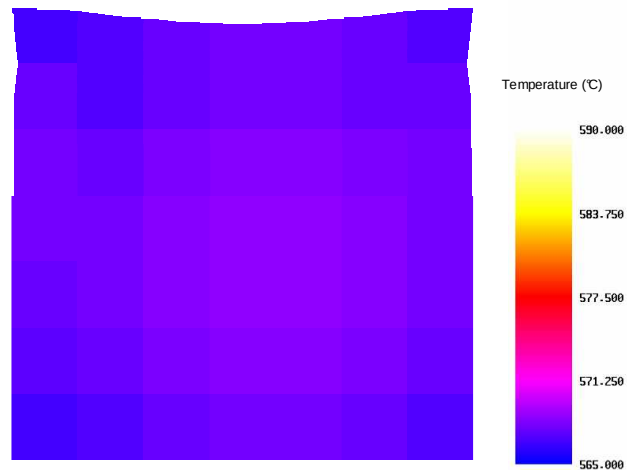


Figure 4.8: Temperature distribution plotted with the free surface contour .

It is not until an average solid fraction of 98 % that a cell meets the criterion. At this moment a number of pores will form at several locations. These pores remain small, because only 2% liquid is left to solidify, i.e., to shrink as showed in Figure 4.9a) Figure 4.9 shows the final shape for both cases, long and short freezing alloys (middle section). Though the total amount of shrinkage is identical, the freezing range was found to have a pronounced effect on the internal or external distribution of porosity. The long freezing range alloy exhibits mainly external porosity and a distributed small internal porosity, where the short freezing range alloy exhibits mainly concentrated internal shrinkage, i.e., one large hole, porosity and the top shape is much more sharp.

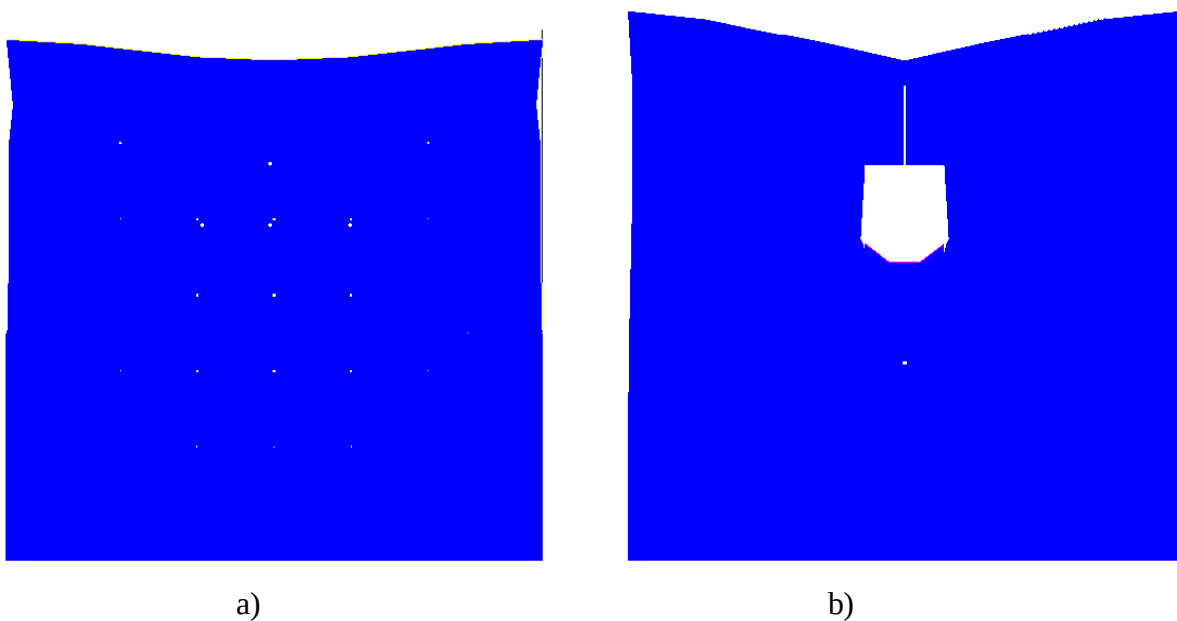


Figure 4.9: Comparison between the final shape in a) short and, b) long freezing material.

A comparison of top surface evolution through solidification is presented in Figure 4.10. The depression of two points, “A” in top middle and “B” in the corner, are plotted. The difference in the top surface shape is clear. The short freezing presents a pronounced depth, whereas the long freezing shows a much flatter surface.

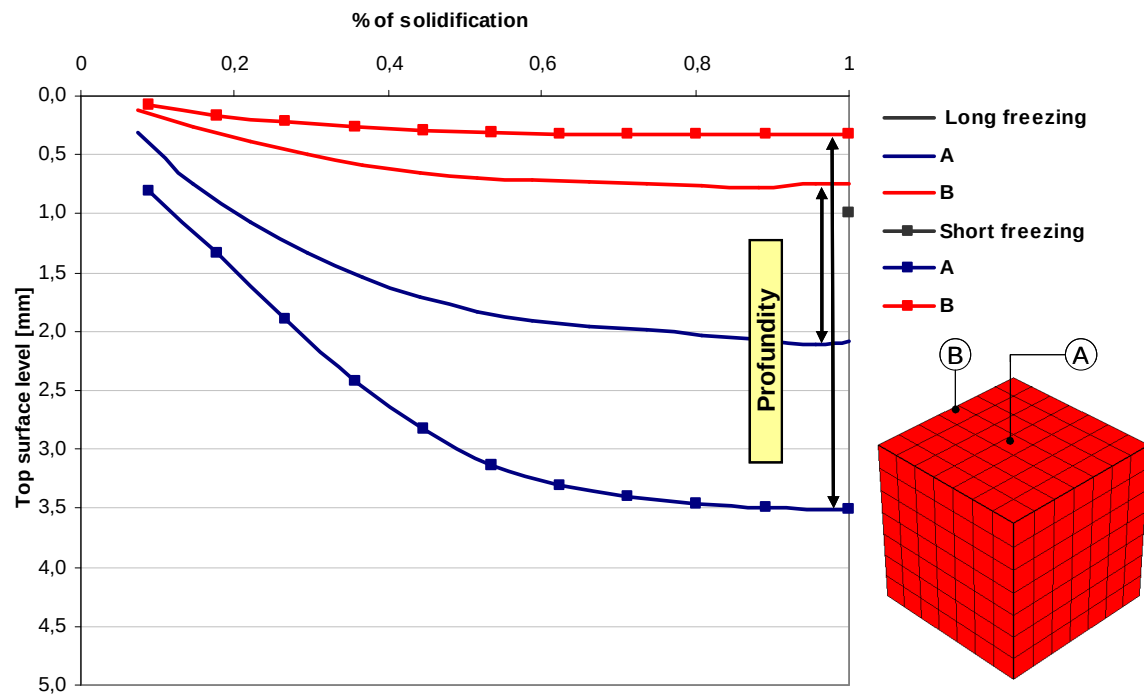


Figure 4.10: Comparison of the top surface evolution for long and short freezing alloys.

4.1.3. Discussion

Figure 4.9 illustrates how the specification of material freezing range can influence the type of porosity predicted by the numerical model. In a short freezing material the outside layers quickly solidify. Therefore, compensating the volume deficit of the shrinking material inside the casting is not possible by movement of the outside layers. The pressure will then quickly drop and the criterion to form a pore is met. However, in a long freezing material the outside layers will remain mushy and are able to compensate shrinkage due to their significantly longer movement as a consequence of their low resistance to inward flow. This results in less porosities formed inside the casting, because most of the shrinkage is already compensated by movement of the outside layers.

As long as the outside layers compensate the volume deficit by solidification, the feeding velocity is directed from the surface to the inside, i.e., the metal is driven by the pressure gradient from the outside to the inside. As soon as a pore is formed the feeding velocity is directed away from the pore to the outside, because the pressure inside the pore is higher than the pressure of the surrounding liquid which is shrinking. This results in a sudden direction change of the velocities when a pore opens. As a result the movement of the surface to the inside immediately stops.

The model shows that pore formation occurs earlier in short freezing range alloys than in long freezing range alloys. The result is that short freezing alloys are more prone to internal shrinkage porosities than long freezing alloys, because more volume deficit due to shrinkage has to be fed from the pores.

4.2 Cup – Validation test case

In this section, the experiment and model validation will be described in some detail Part of the work reported took place at SIRRIIS (the Collective Centre for the Belgian Technological Industry).

4.2.1. Cup experiment

Two typically aluminium alloys used in casting, AlSi7 and AlSi12 were selected. The first alloy, AlSi7 can be considered as a long freezing one, Figure 4.14. The AlSi12 is considered as a short freezing one (almost eutectic composition), Figure 4.15. Data for solidification curves were acquired and used latter-on in the numerical validation.

The setup for this experimental test is showed in Figure 4.11 to Figure 4.13.

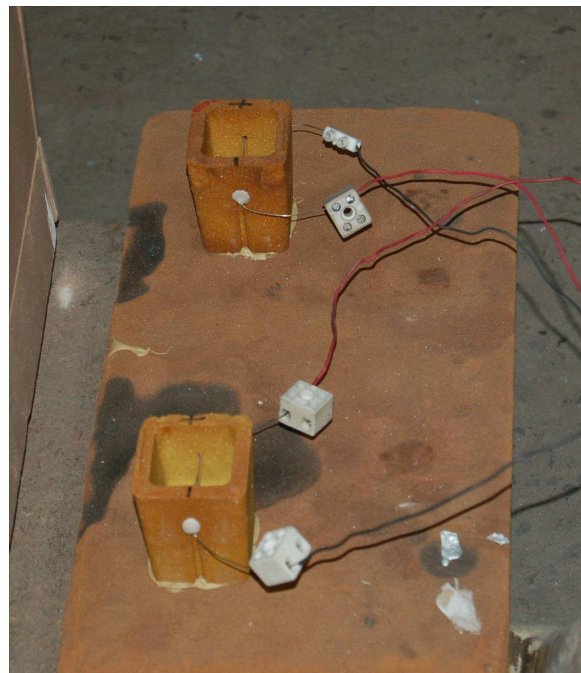


Figure 4.11: Casting with a data acquisition system (cooling curves).

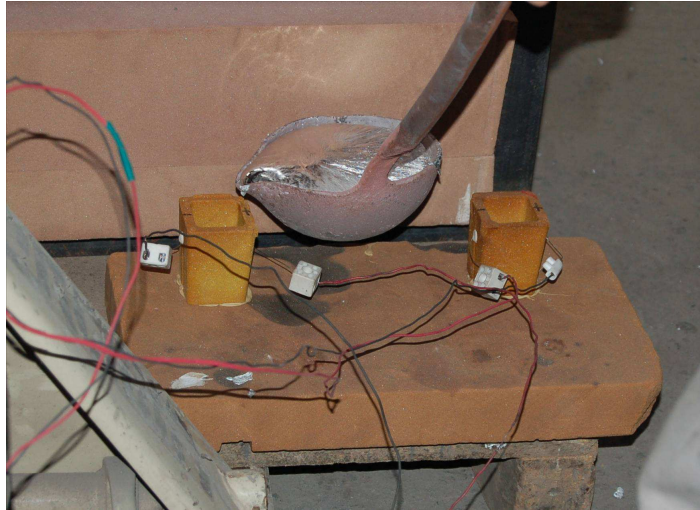


Figure 4.12 – Pouring.

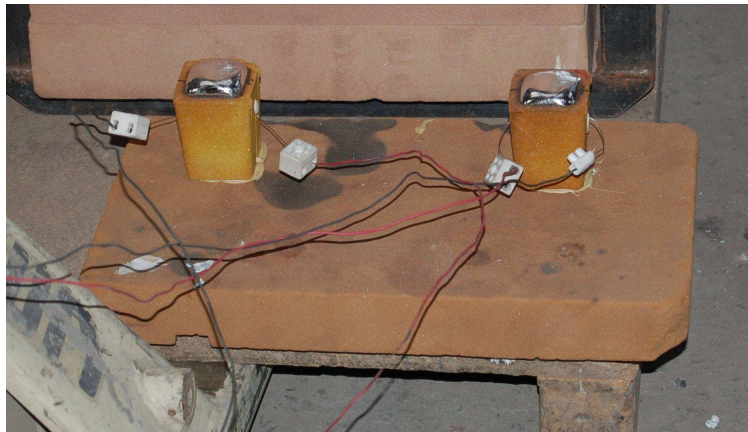


Figure 4.13: Solidification, final stage.

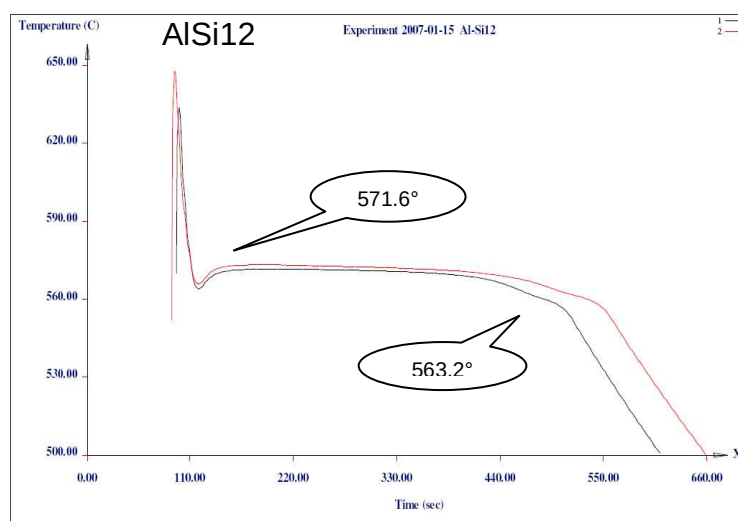


Figure 4.14: Experimental cooling curve for AlSi12 alloy.

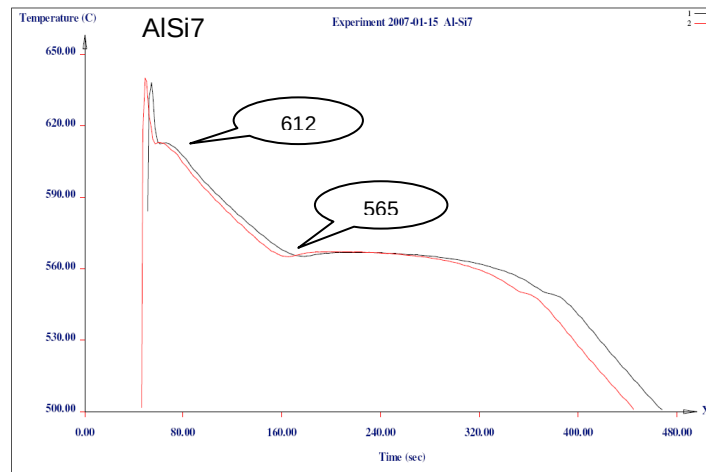


Figure 4.15: Experimental cooling curve for AlSi7 alloy.

The samples were sectioned and polished as shown in Figure 4.16 and Figure 4.17. The shapes revealed several forms of shrinkage defects. The different top geometry obtained in each alloy is quite obvious. In case of AlSi12 the top surface presents a pronounced central shrinkage whereas the AlSi7 has a much flatter surface. Also some internal porosity is visible in both alloys. In the AlSi7 this porosity is smaller and more uniformly distributed.



Figure 4.16: Sectioned sample AlSi12.



Figure 4.17: Sectioned sample AlSi7.

4.2.2. Parameterizing the computational model — key issues

While most of the material properties for the flow and heat-transfer aspects of the model can be identified from the literature (and the relevant data here are summarized in Chapter 2), the key parameters for the shrinkage porosity model, the porosity initiation pressure, P_{crit} , below which voids are assumed to nucleate within the liquid phase, and the permeability coefficient K_0 , which characterizes the flow resistance of the mushy zone are all unknown. These are functions of a number of parameters, including the local liquid fraction, dendrite size, structure and its distribution, and they are difficult to quantify without further expensive experiments. For this reason, a parametric variation of these quantities was performed in a three dimensional simple shape. The influence of the freezing interval and mesh size is also analyzed.

A three-dimensional model of the filled cavity, with dimensions as indicated in Figure 4.18, is considered. The numerical model is also shown. The mesh has a total of 7942 elements: 490 of which are metal and the remaining are sand.

The analysis performed included heat transfer and solidification with feeding flow model where all boundaries are free surfaces. The cavity is considered to be filled at the beginning of simulation. Again, the objective was to:

- identify a parametric range for the permeability coefficient constant, K_0 ;
- establish a porosity critical pressure/criteria, P_{crit} , that could be used in complex shape casting simulations;
- the influence of solidification interval;
- mesh sensitivity.

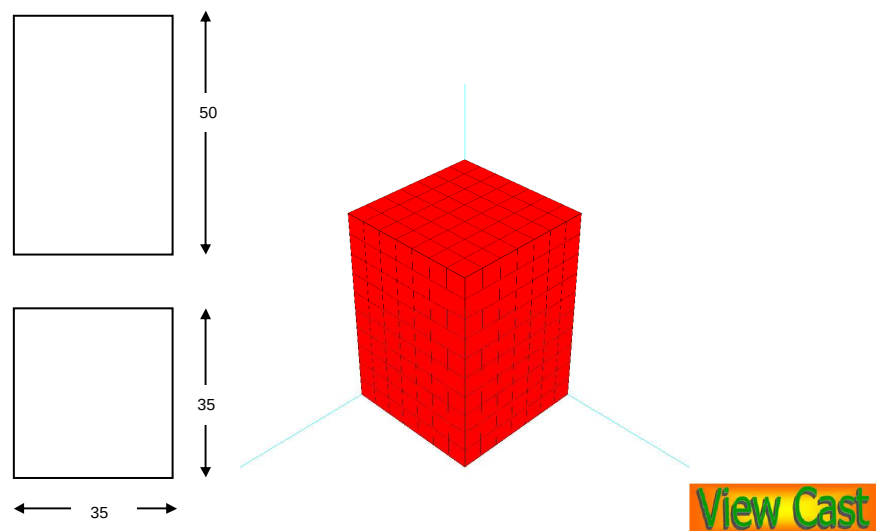


Figure 4.18: Geometrical and numerical model for parameterizing the computational model.

The numerical parameters used in discretisation are presented in Table 4.1. Table 4.2 presents the number of time steps and CPU time needed for each material.

Table 4.1: Numerical parameters.

	dx	dy	dz	n° of elements	Time step
metal		5mm		2451	0.001s
sand		5-30mm		3726	

Table 4.2: Number of time steps and CPU time

	n° time steps	CPU time
AlSi12	90135	1350s
AlSi7	90005	4500

4.2.2.1. The effect of permeability

Simulations were carried out for a range of values for the permeability constant, K_0 , over a range $K_0=2.8E-10$ to $2.8E-12$. A fixed value, $2.8E-10$, is used before the solid fraction equals 0.3 (chapter 2, section 2.4). When a columnar solidification is considered, the permeability has a constant value of $2.8E-13$. The results are shown for three different cases:

$$\begin{array}{l} \text{CASE I} \left\{ \begin{array}{ll} E-10 & \text{if } f_s < 0.3 \\ \mathbf{E-10} & \text{if } \mathbf{f_s > 0.3} \\ E-13 & \text{if columnar} \end{array} \right. \quad \text{CASE II} \left\{ \begin{array}{ll} E-10 & \text{if } f_s < 0.3 \\ \mathbf{E-11} & \text{if } \mathbf{f_s > 0.3} \\ E-13 & \text{if columnar} \end{array} \right. \quad \text{CASE III} \left\{ \begin{array}{ll} E-10 & \text{if } f_s < 0.3 \\ \mathbf{E-12} & \text{if } \mathbf{f_s > 0.3} \\ E-13 & \text{if columnar} \end{array} \right. \end{array}$$

a) AlSi12 (short freezing alloy)

In Figure 4.19 to Figure 4.21 results of the effect of the permeability coefficient on porosity predictions are shown for the three cases. The colour contour indicates the level of porosity and next the upper free surface profile is presented. To plot this profile the average value of VOF of each element is considered.

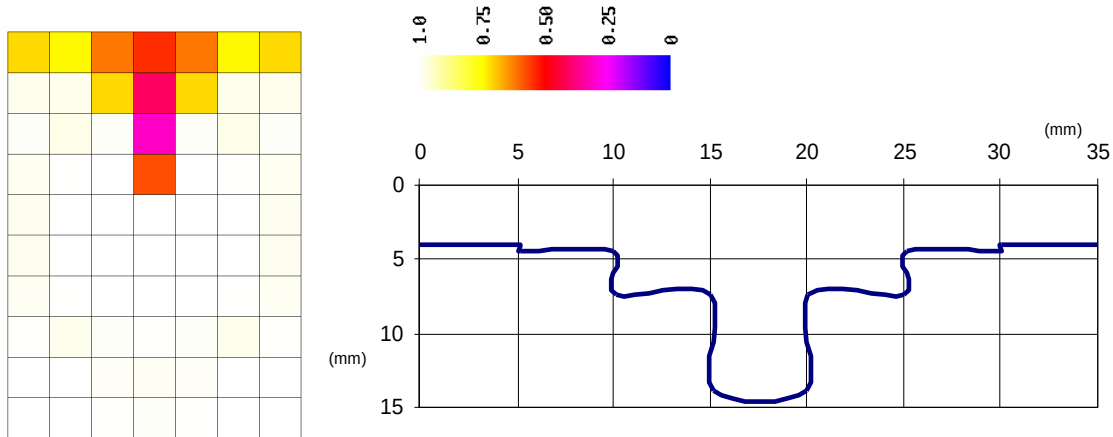


Figure 4.19: Porosity contour and top free surface profile, case I.

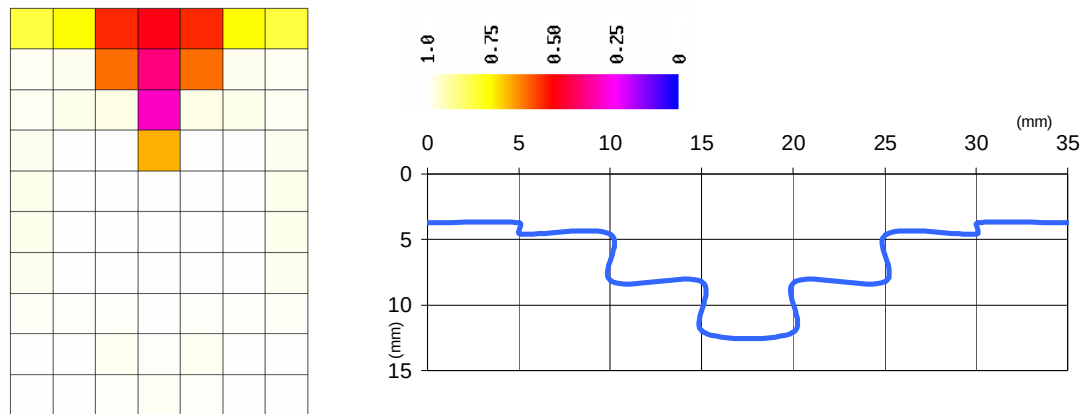


Figure 4.20: Porosity contour and top free surface profile, case II.

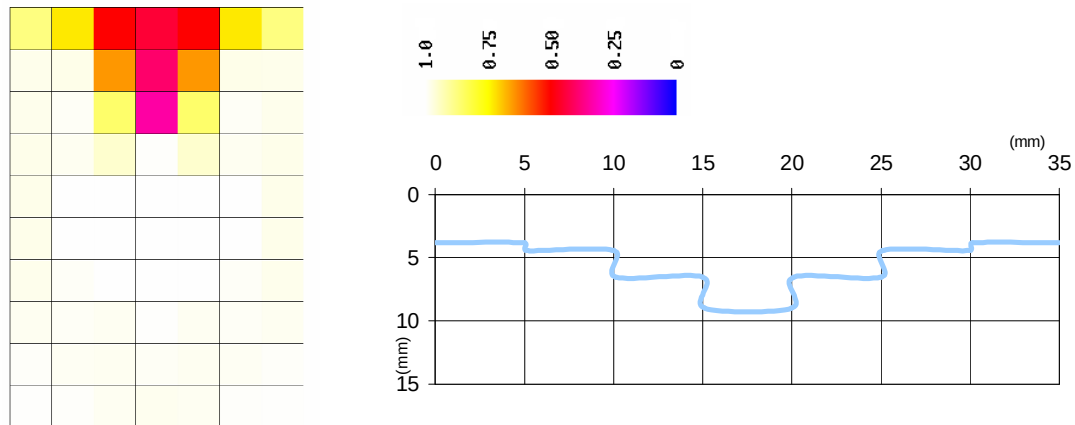


Figure 4.21: Porosity contour and top free surface profile, case III.

The upper surface profile shows a deep slope in the centre that decreases as the permeability coefficient decreases.

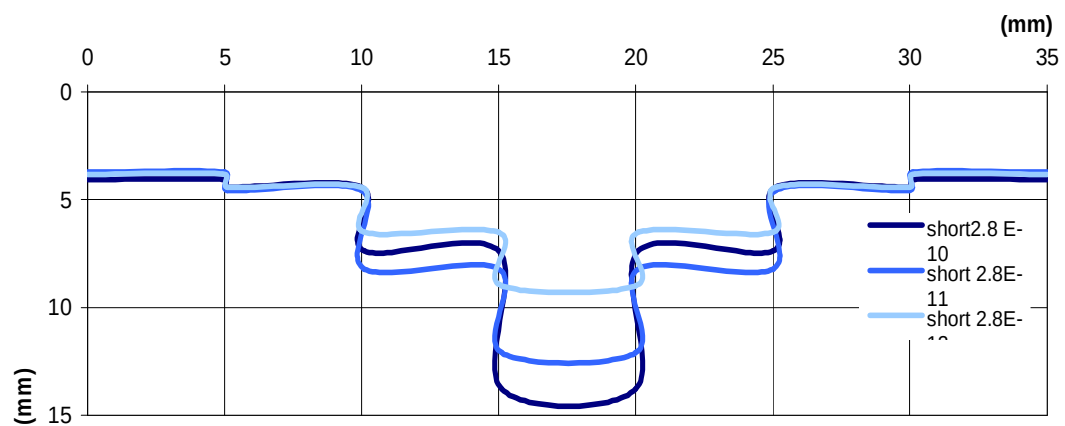


Figure 4.22: Comparison of the different surface profiles obtained in short freezing alloy, AlSi12.

In Figure 4.23 the amount of each type of defect found in the three cases is compared. The types of defect quantified are: pipe shrinkage corresponding to the upper surface shrinkage; sink, which represents the wall depression; and void representing internal porosity. The pipe shrinkage is higher for a higher K_0 . On the other hand the amount of the other type of defects considered (sinks and voids) increases as the permeability coefficient decreases.

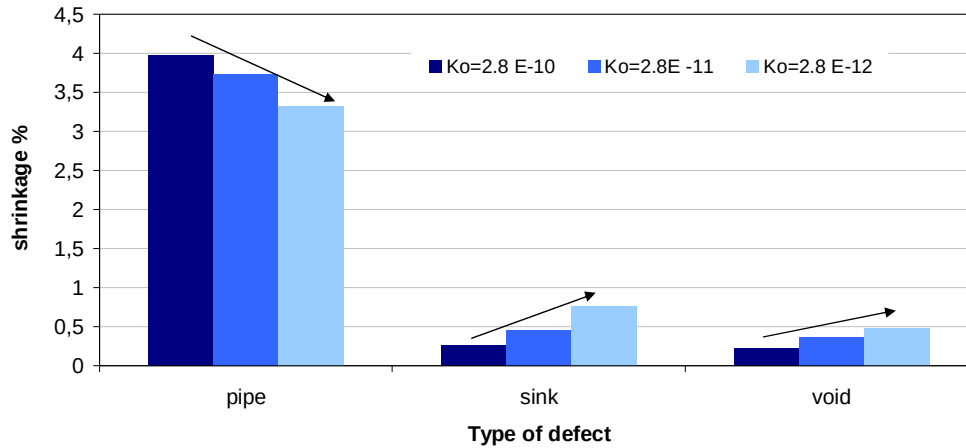


Figure 4.23: Distribution of defects for each K_0 .

In Figure 4.24 the three cases are compared in terms of defects distribution. For a higher permeability coefficient, the shrinkage defects are concentrated in the form of pipes (case I). Increasing K_0 the pipe shrinkage decreases which is compensated by an increasing amount of the other defects, sinks and internal voids.

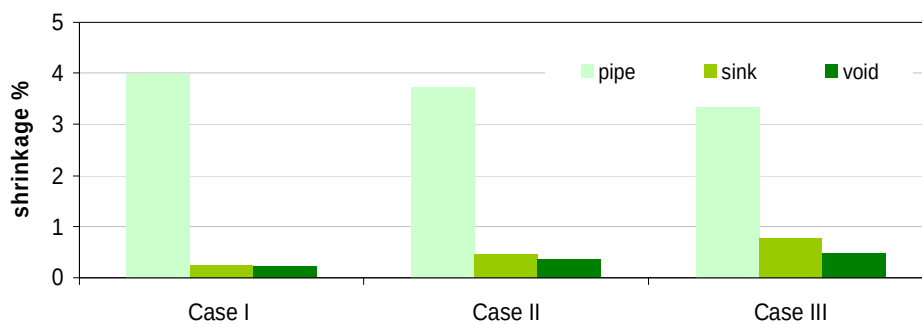


Figure 4.24: Distribution of defects in the three cases.

b) Long Freezing alloy(AlSi7)

In Figure 4.25 to Figure 4.27 results of the effect of permeability coefficient on porosity predictions are shown for the three cases.

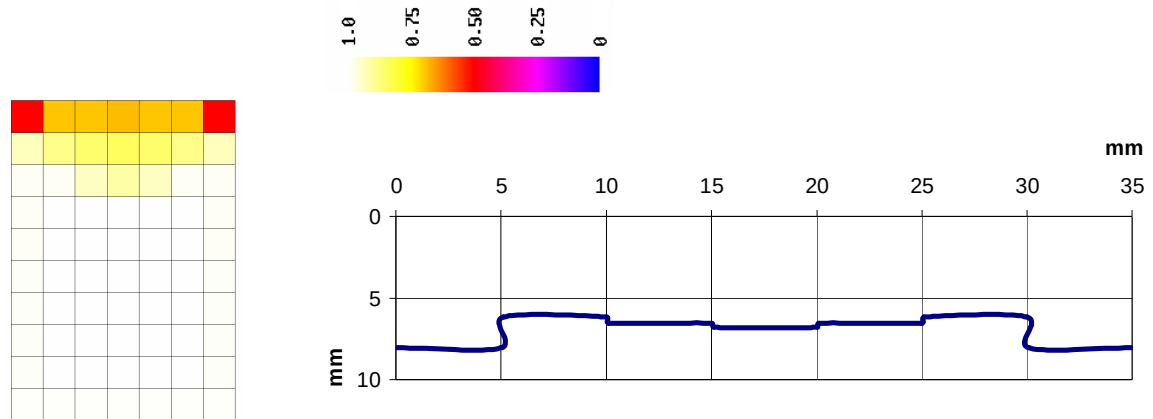


Figure 4.25: Porosity contour and top free surface profile, case I.

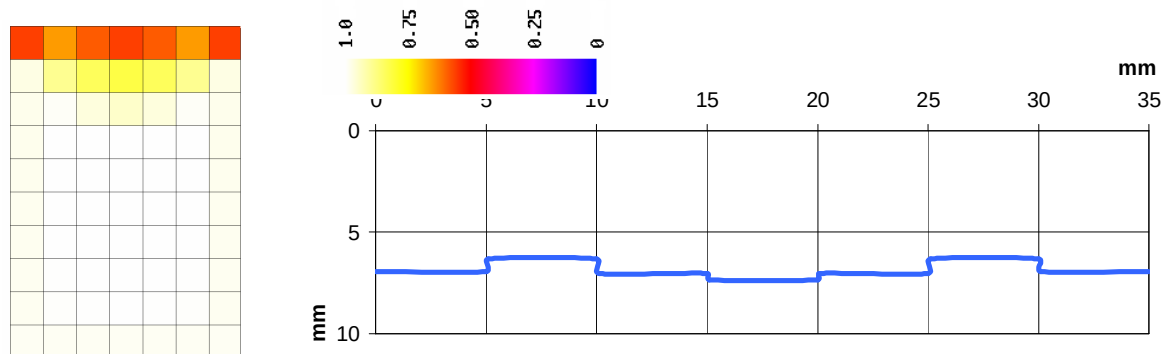


Figure 4.26: Porosity contour and top free surface profile, case II.

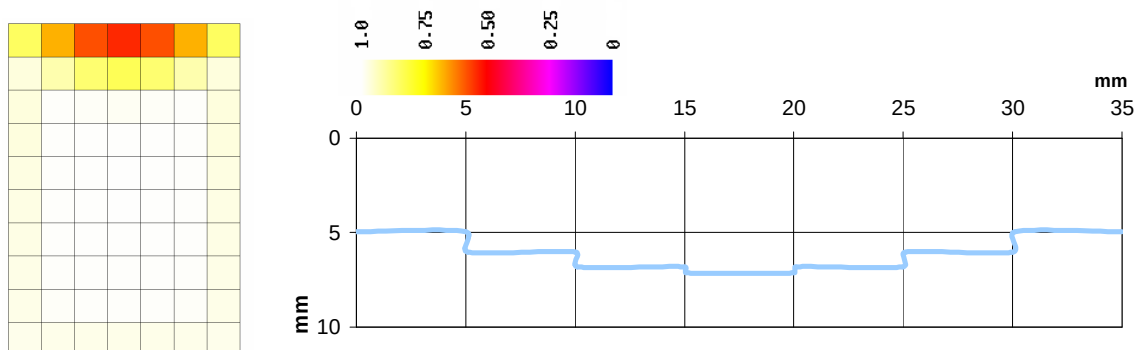


Figure 4.27: Porosity contour and top free surface profile, case III.

The upper surface profile doesn't show a significant slope in the centre, as previously found in the AlSi12 alloy, but shows a much more uniform surface. The decrease of the decreasing amount of pipe shrinkage defects with decreasing permeability was also evident, Figure 4.29. In addition, the wall defects and internal porosity are superior as K_0 decreases. Figure 4.29 shows the amount of each type of defect found in the three cases.

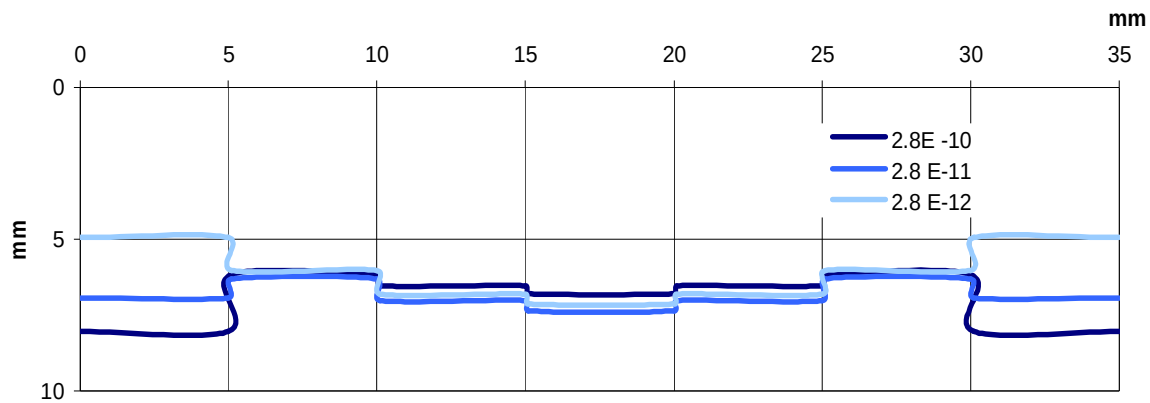


Figure 4.28: Comparison of the different surface profiles obtained in the long freezing alloy, AlSi7.

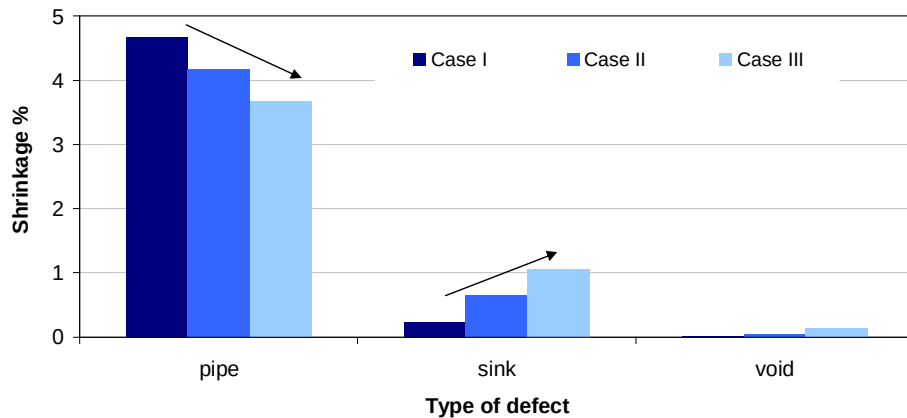


Figure 4.29: Distribution of defects for each K_0 .

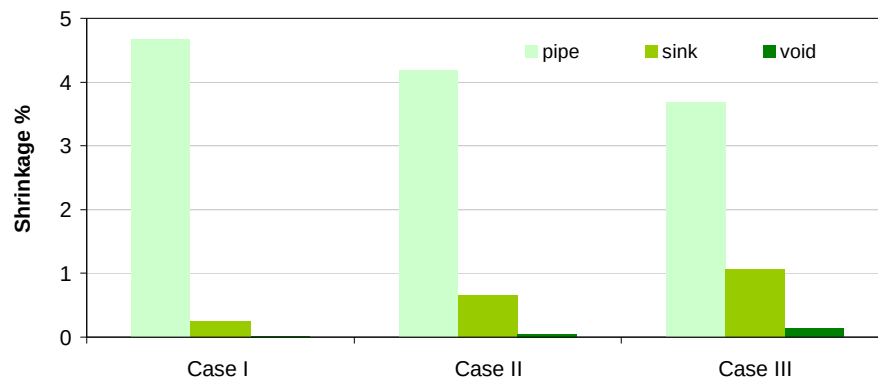


Figure 4.30: Distribution of defects in the three cases.

Key point

It is clear that permeability has a significant influence on the macroporosity/void formation as might be expected. For a high permeability, the metal can flow to feed the solidifying areas sufficiently well to avoid the depression in the upper level, or as in long freezing alloy to avoid the shrinkage in the form of sinking of the walls. However, for low permeability, the feeding flow from upper level is severely restricted resulting in a more profound depth in the top for the AlSi12, and in AlSi7 this is revealed in sinking of the wall.

4.2.2.2. Freezing interval

This section intends to show the ability of the model to represent the differences found in the two types of alloys.

Figure 4.31 and Figure 4.32 compare results of case II (section 4.1, page 108) for each alloy, AlSi12 and AlSi7. These results show that the difference in the top surface shape is clear. The short freezing presents a pronounced depth, whereas the long freezing shows a much flatter surface.

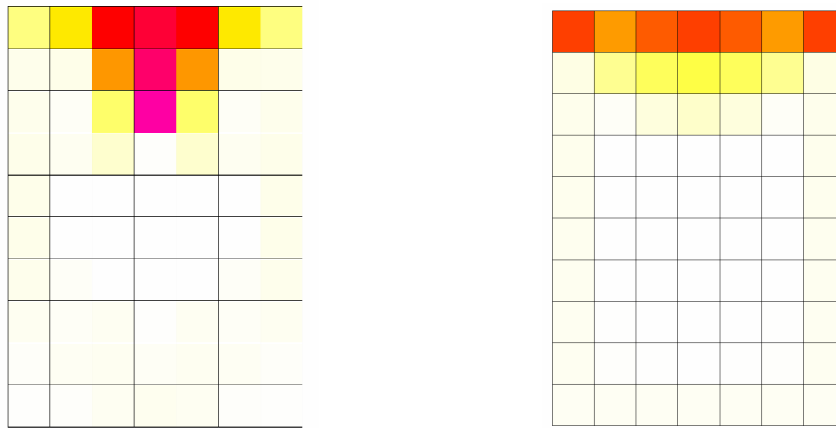


Figure 4.31: Porosity contour obtained in case II in AlSi12 and AlSi7.

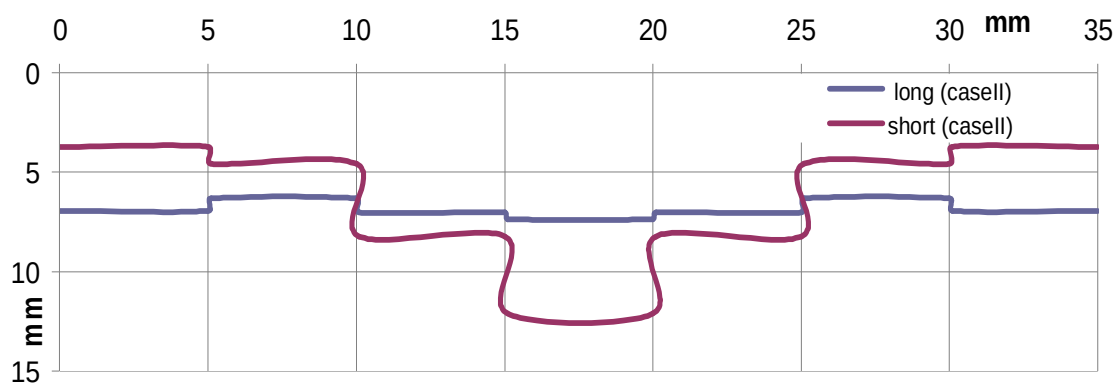


Figure 4.32: Comparison of the free surface profile, case II.

As already stated in a long freezing material the outside layers remain mushy for a longer time and are able to compensate the shrinkage by sinking of the surfaces, Figure 4.34. This

results in less shrinkage porosities (Figure 4.35) formed in the inside of the casting, since the greater part of the shrinkage is already compensated by the movement of the outside layers. In a short freezing material the outside layers quickly solidify. Therefore, compensating the volume deficit of the shrinking material has to come from the opening of voids.

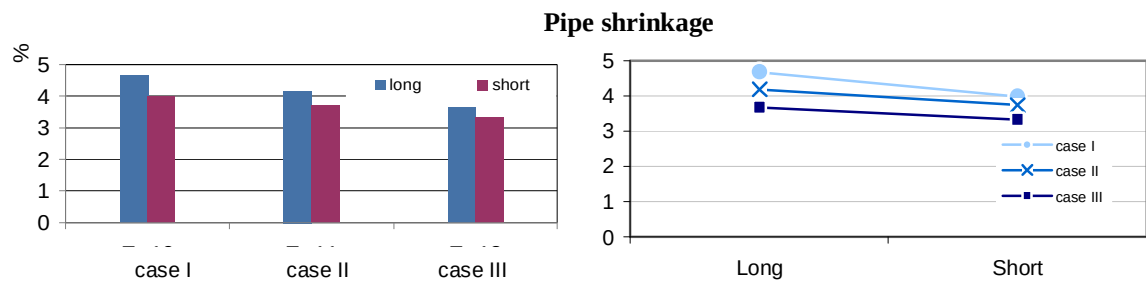


Figure 4.33: Comparison of pipe shrinkage in AlSi7 and AlSi12 in case I, II and III.

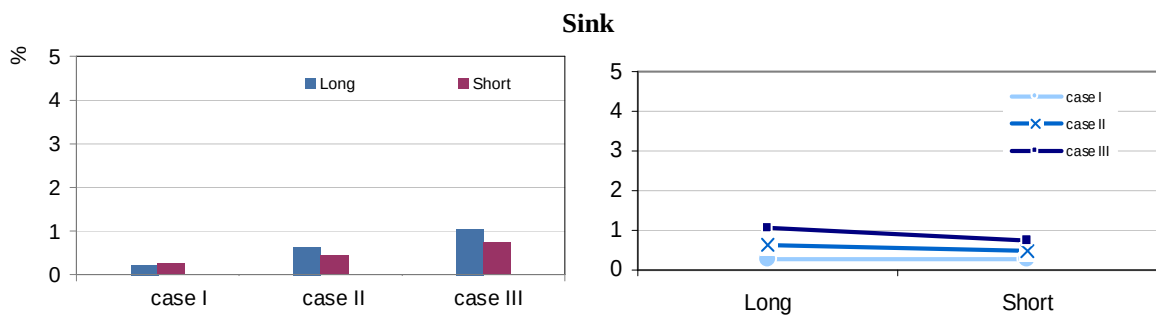


Figure 4.34: Comparison of sink shrinkage in AlSi7 and AlSi12 in case I, II and III.

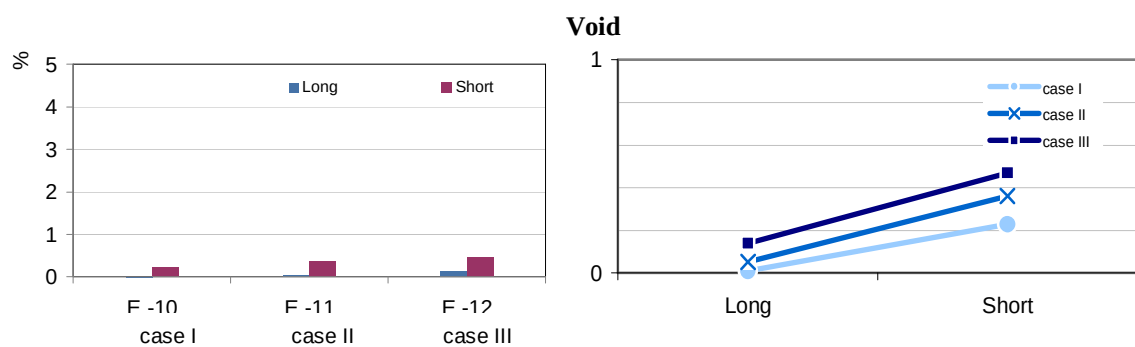


Figure 4.35: Comparison of void shrinkage in AlSi7 and AlSi12 in case I, II and III.

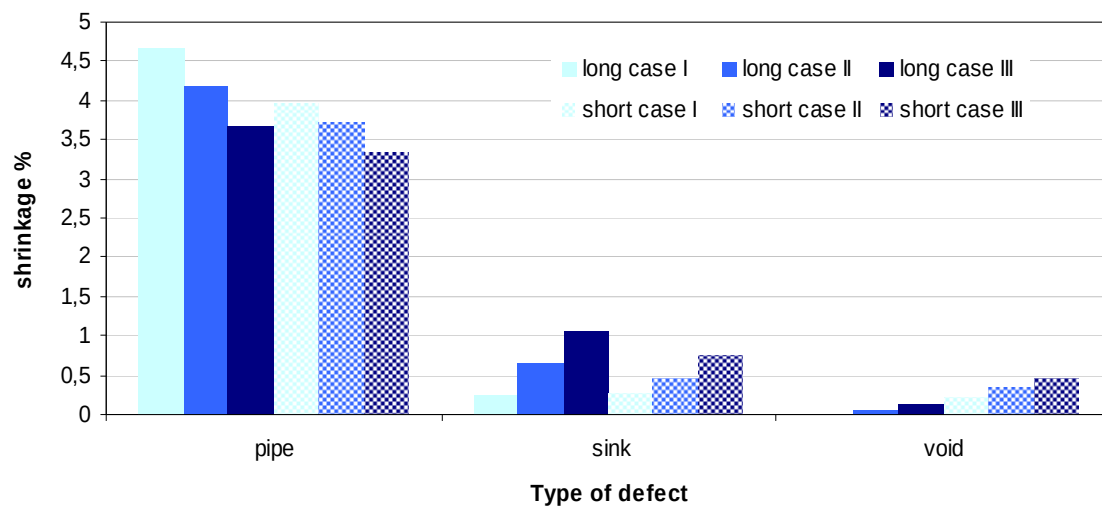


Figure 4.36: Comparison of all type of defects in AlSi7 and AlSi12 in case I, II and III.

4.2.2.3. Boundary condition

In this section the effect of the boundary condition considered for free surfaces (established in chapter 2) is tested. This boundary condition consists in considering for free surfaces and after coherency, $fs > 0.3$, permeability coefficient takes a lower value (less permeability) in perpendicular direction along a critical thickness.

Three scenarios are considered, Table 4.2. In all three permeability takes the value of $2.8E^{-11}$ but each one has different condition at surface when $fs > 0.3$. The first situation assumes a constant permeability coefficient through all solidification, i.e., no special boundary condition. In the second scenario a ten times smaller for K_0 is considered at the surface after coherency fraction (0.3). In the third situation one hundred times smaller value is taken. (This 3rd scenario corresponds to case II analyzed in previous section.

Table 4.2: Three scenarios for boundary conditions.

1 st scenario : no different boundary condition is set:	
	$K_0 = 2.8E^{-11}$
	at free surface after coherency ($fs > 0.3$)
	$K_0^{\text{free surf.}} = K_0 = 2.8E^{-11}$
2 nd scenario : 10× lower $k_0^{\text{free surf.}}$:	
	$K_0 = 2.8E^{-11}$
	at free surface after coherency ($fs > 0.3$)
	$K_0^{\text{free surf.}} = 2.8E^{-12}$
3 rd scenario : 100× lower $k_0^{\text{free surf.}}$:	
	$K_0 = 2.8E^{-11}$
	at free surface after coherency ($fs > 0.3$)
	$K_0^{\text{free surf.}} = 2.8E^{-13}$

The results for the porosity contour and the top free surface profile are presented in Figure 4.37 to Figure 4.39 each corresponding to the scenarios defined.

1st scenario no condition is set:

$$K_0^{\text{free surf.}} = K_0 = 2.8E-11$$

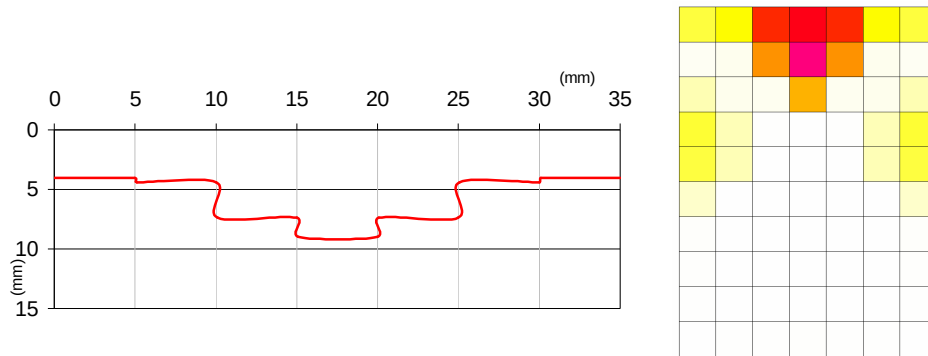


Figure 4.37: Porosity contour and top free surface profile, 1st scenario.

2nd scenario 10X lower permeability:

$$K_0^{\text{free surf.}} = 2.8E-12; K_0 = 2.8E-11$$

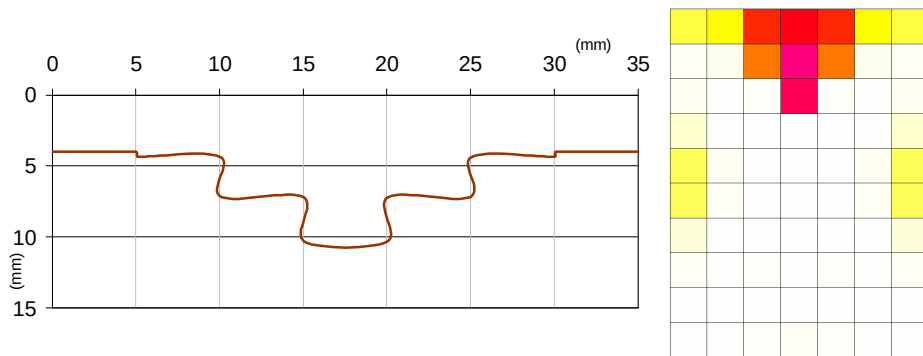


Figure 4.38: Porosity contour and top free surface profile, 2nd scenario.

3rd scenario 100x lower value:

$$K_0^{\text{free surf.}} = 2.8E-13; K_0 = 2.8E-11$$

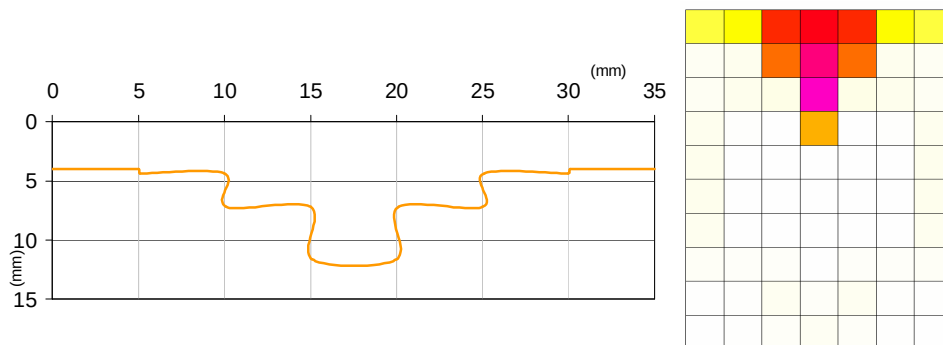


Figure 4.39: Porosity contour and top free surface profile, 3rd scenario.

As expected, this boundary condition has a clear influence on results. When no condition is set, Figure 4.37, the slop in the top is less pronounced and the shrinkage is compensated by depression of the other free surfaces, sink defect. This is explained because the free surfaces keep the ability to feed solidification shrinkage through all solidification. If this condition is introduced the ability to feed shrinkage trough the free surface decreases, as observed in Figure 4.38 and Figure 4.39.

In Figure 4.40 the three obtained profiles are compared.

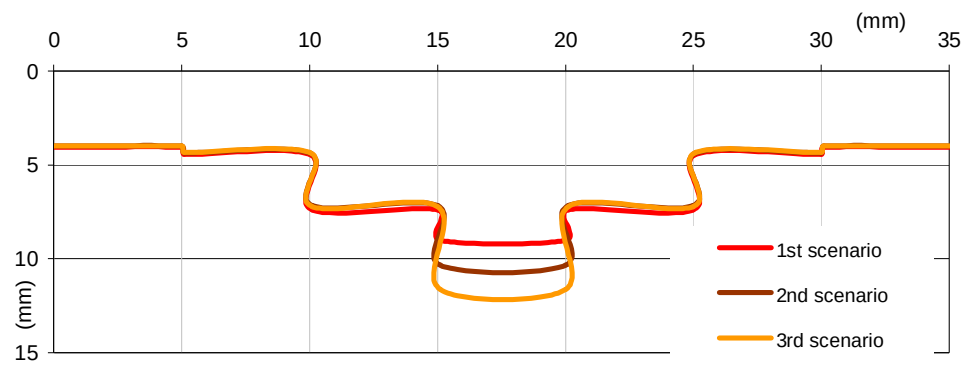


Figure 4.40: Comparison of top free surface profile for the three scenarios.

4.2.2.4. The impact of the initiation pressure

Several pressure criteria were tested:

- P₁) $P_{crit} = P_{cavitation}$ In general, the cavitation pressure of liquid metals at casting temperature is very small. At casting temperatures around 750°C, the cavitation pressure for pure aluminium was determined from published data [Handbook of Chemistry and Physics, 1989] to be approximately 10 Pa;
- P₂) small pressure drop (5000 Pa);
- P₃) $P_{crit} = F(fs)$ Several linear functions where the critical pressure is a function of the solid fraction are considered. Although this work only considers the shrinkage porosity this type of criterion is justified when hydrogen or inclusion contribution is considered. The hydrogen is dissolved in the metal at the moment the solidification starts. At a first moment the hydrogen is entrapped in the growing solid phase and subsequently rejected to melt. The solid solubility of many elements in the solid phase is considerably lower than in the liquid phase, as such the components of an intermetallic are driven out from the solid phase in to the melt and can enrich there. Due to the increased activity of the reaction partners, the intermetallic can be formed.

The critical pressure parameter, P_{crit} , had a minor influence on the obtained results and the corresponding plots were quite identical. This should be explained by the fact that when the pressure starts to drop, then it falls abruptly (almost asymptotic) and any value of P_{crit} is inevitably reached.

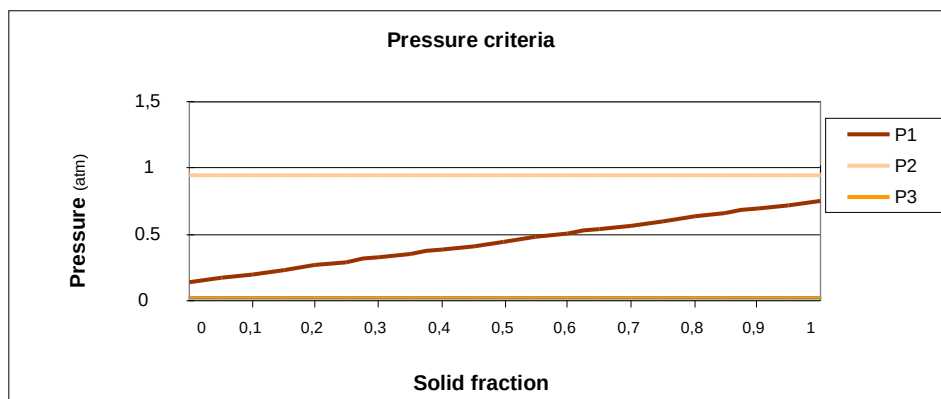


Figure 4.41: Pressure criteria tested.

4.2.2.5. Mesh sensitivity

An analysis for mesh sensitivity was carried out for case II and for both materials (section 4.2.2.1, page 108). Results for two uniform meshes ($dx=dy=dz$) one with 2.5 cell size and the other with 5mm cell size are presented.

$$CASE\ II \left\{ \begin{array}{ll} E-10 & \text{if } f_s < 0.3 \\ E-11 & \text{if } f_s > 0.3 \\ E-13 & \text{if columnar} \end{array} \right.$$

a. AlSi12, short freezing alloy

Figure 4.42 shows a comparison of top free surface profile obtained with each different mesh. No significant difference was found.

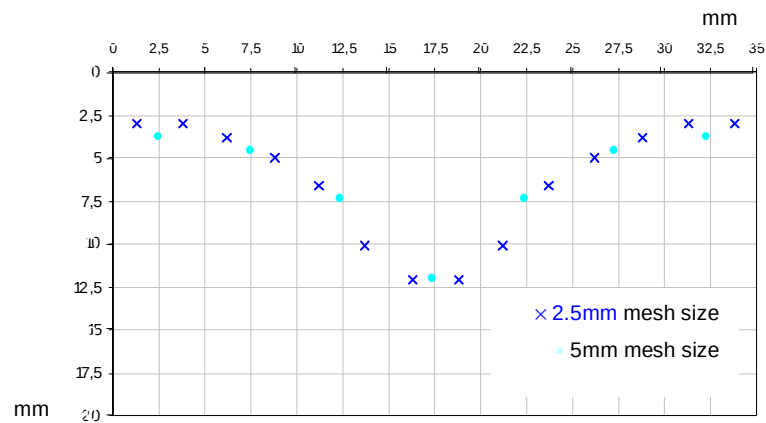


Figure 4.42: Comparison of top free surface profile obtained with a mesh of 2.5mm and 5mm in AlSi12.

In Figure 4.43 the results obtained with the two meshes are compared, for each defect considered. The difference, as percentage of the total shrinkage, is also displayed.

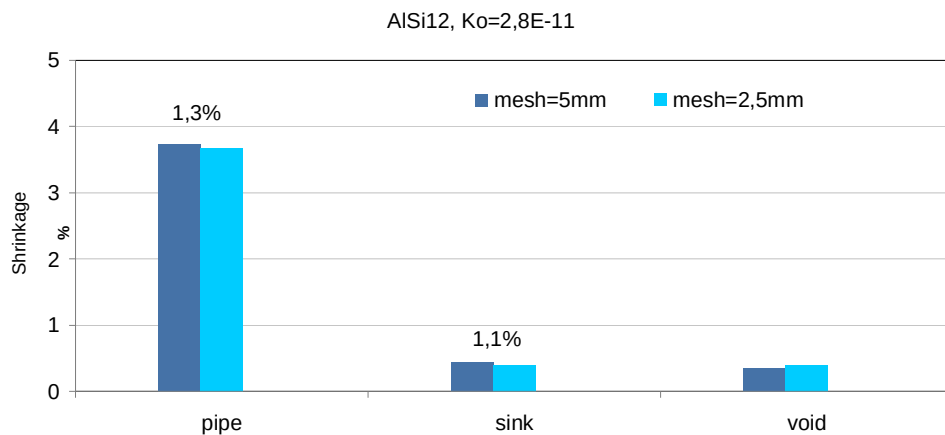


Figure 4.43: Difference between result of the amount of each type with a 2.5 and 5mm mesh.

From Figure 4.43, the differences found in the two mesh results can't be considered significant.

b. AlSi7, long freezing alloy

Figure 4.44 shows a comparison of top free surface profile for the long freezing AlSi7. The long freezing alloy seems less sensitive to mesh dimension where compared with the short freezing material.

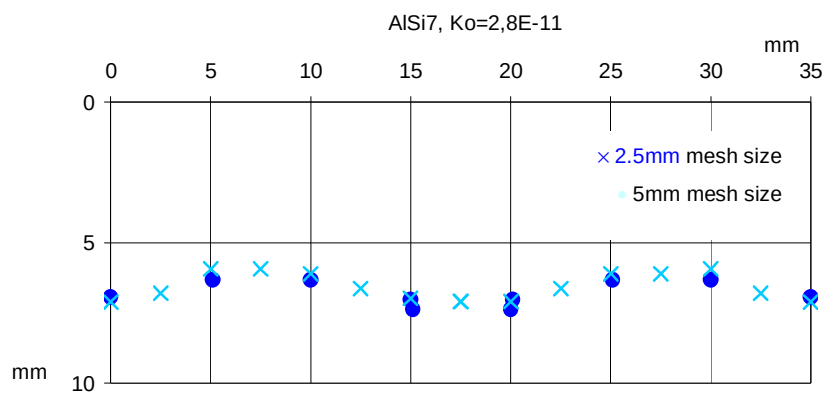


Figure 4.44: Comparison of top free surface profile obtained with a mesh of 2.5mm and 5mm in AlSi7.

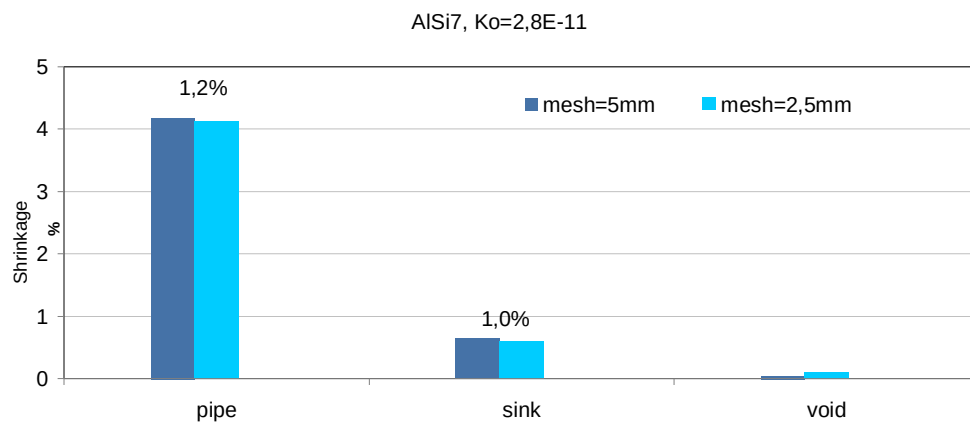


Figure 4.45: Difference between result of the amount of each type with a 2.5 and 5mm mesh.

Also, as in AISi12, the differences found in the distribution of the defects aren't significant.

4.2.3. Experimental results

In this section the experimental results are compared, with different numerical results obtained in section 4.1, in order to find the best fitting situation.

a. AlSi12 – Short freezing alloy

In Figure 4.46 the top section profile for the AlSi12 is compared with results presented in section 4.2.2.1 for the three cases.

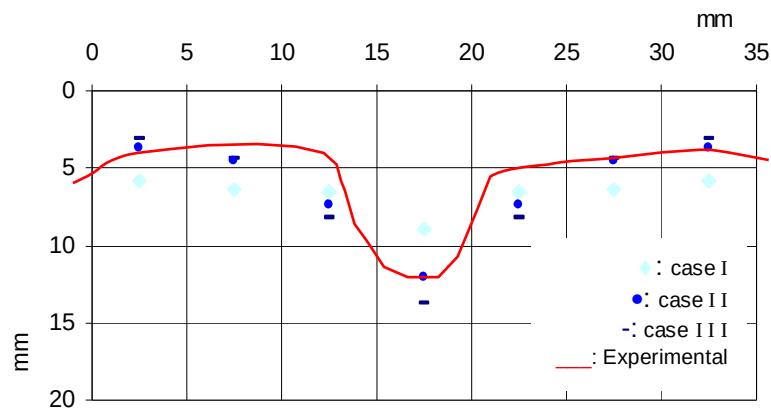


Figure 4.46: Comparison between the experimental shape, red line, and numerical results (case I, II and III) for AlSi12.

The results in Figure 4.46 show that numerical results resemble the experimental one. The Case II is closer with the experimental profile.

b. AlSi7 – Long freezing alloy

In Figure 4.47 the experimental shape of AlSi7, long freezing alloy, is compared with numerical results.

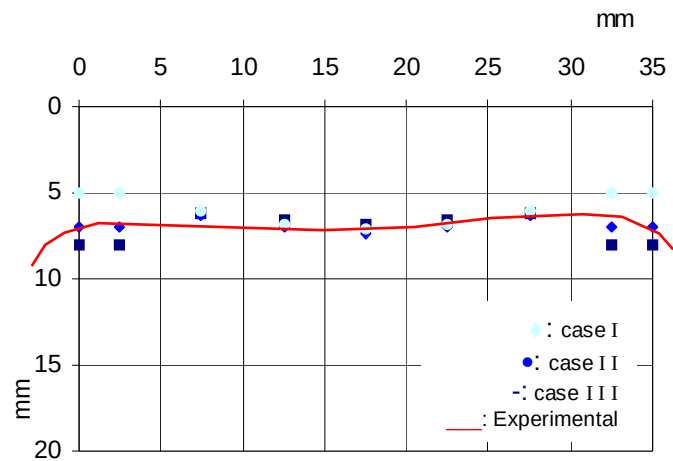


Figure 4.47: Comparison between the experimental shape and the numerical profiles (case I, II and III) for AlSi7.

Also for the long freezing alloy, AlSi7, the results showed good reproducibility of the experimental shape.

Key points

The results shows internal and outside shrinkage defects depending on the freezing range of the metal. The expected shrinkage features are well described by the current model.

An extensive sensitivity analysis was carried out, in which many other simulations were actually performed with a range of the parameter, K_0 and P_{crit} , sets. However, it became quickly apparent what was the appropriate parameter range that adequately reflected the main experimental observations.

- The permeability coefficient, K_0 , was found to have a great influence in the model.
- The critical pressure parameter, P_{crit} , had a minor influence on the obtained results and the corresponding plots were quite identical. This should be explained by the fact that when the pressure starts to drop, then it falls abruptly (almost asymptotic) and any value of P_{crit} is reached after a few time steps.

CHAPTER 5

CASTING OF A 3D COMPLEX SHAPE

The computer model developed is used to perform real simulations. Experimental work is described. The simulations are compared with the experimental results and the efficiency of the model is discussed.

5.1 Geometry

When designing the geometry for the test case the idea has been to reproduce a real casting condition (set up), while at the same time maintaining the geometry as simple as possible. With a simple geometry we can better identify the variables directly involved in the shrinkage feeding. The choice of the geometry has also been related with the possibility of creating different types of shrinkage defects to illustrate the features of the developed model. Figure 5.1 and Figure 5.2 shows the geometry proposed. This geometry is composed of a feeding system with different cross section connected to metal blocks. The sections are square with dimensions; 14, 16, 18, and 20mm.

5.2 Pouring conditions

Two aluminium alloys, AlSi12 and AlSi7 (a short freezing and a long freezing alloy), were poured, (characterized in section 4.2.1) in a sand mould. The metal was poured at 700°C. Before being poured the alloys were degassed. This treatment was performed by the addition of $0.3\text{NaCl}+2.5\text{AlFe}_3$.

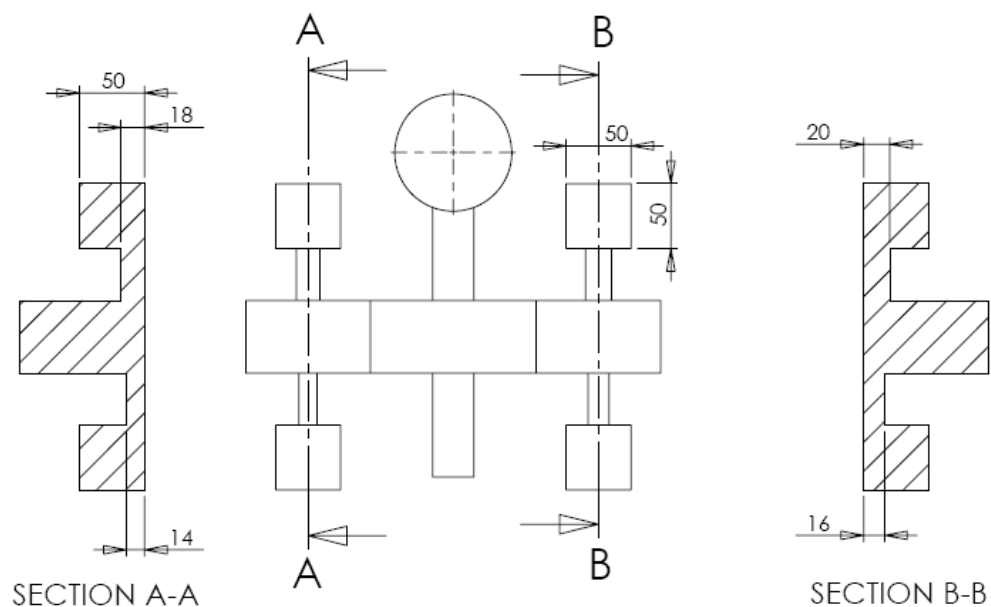


Figure 5.1: Designed geometry, top view and two sections views A-A and B-B.

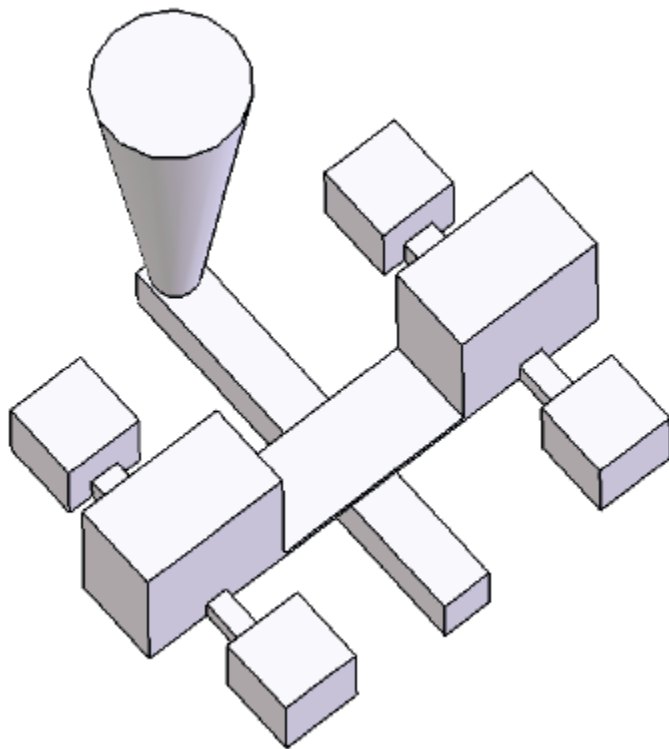


Figure 5.2: 3D model.

To guarantee repeatability, two castings were poured at the same time, Figure 5.3. Figure 5.4 present the obtained components. The samples were cut and polished.



Figure 5.3: Pouring a casting.



Figure 5.4: Castings obtained.

5.3 Experimental results

The castings were cut in two parts. A part with 14 and 18 mm neck and another with 16 and 20 mm neck. Then, samples were cut, section A-A and B-B, and polished.

This section presents results for the two tests performed at the same time (I and II) for each material. Results are presented for both sides of the cuts. A detailed analysis of the shrinkage defects found are presented.

5.3.1. AlSi12

In this section results for the short freezing alloy, AlSi12 are presented.

5.3.1.1. AlSi12, sections 14 and 18mm

Figure 5.5 and Figure 5.6 present the middle cut section A-A, for the two castings poured, test I and II respectively (poured at the same time).

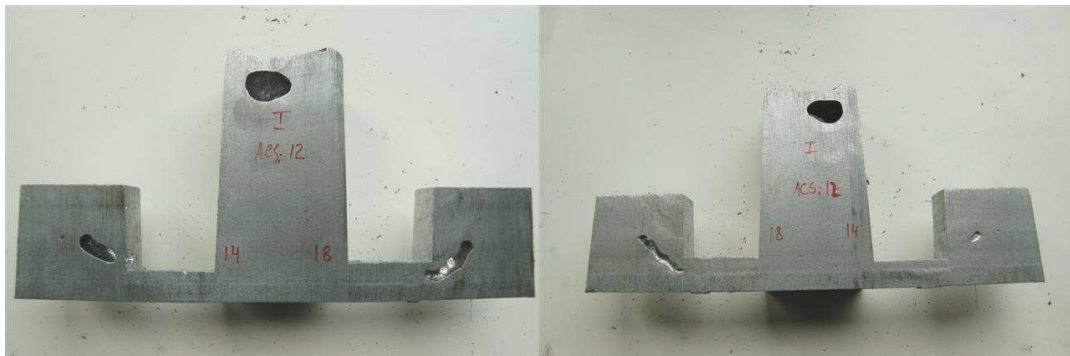


Figure 5.5: AlSi12, short freezing alloy, 14 and 18 mm sections, test I.

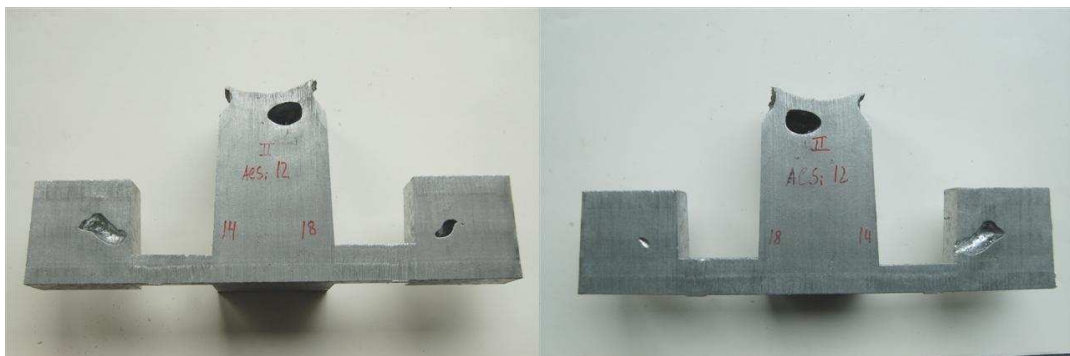


Figure 5.6: AlSi12, short freezing alloy, 14 and 18 mm sections, test II.

5.3.1.2. AlSi12, sections 16 and 20 mm

Figure 5.7 and Figure 5.8 present the middle cut, section B-B, for the two poured castings, test I and II respectively (poured at same time).

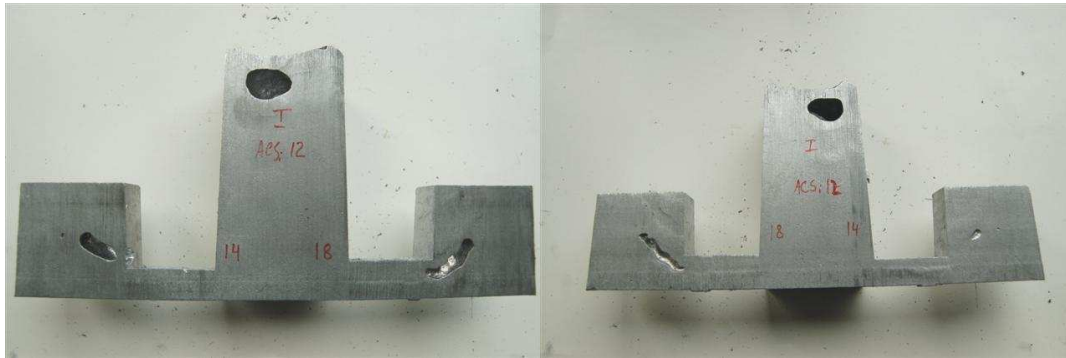


Figure 5.7: AlSi12, short freezing alloy, 16 and 20 mm sections, test I.

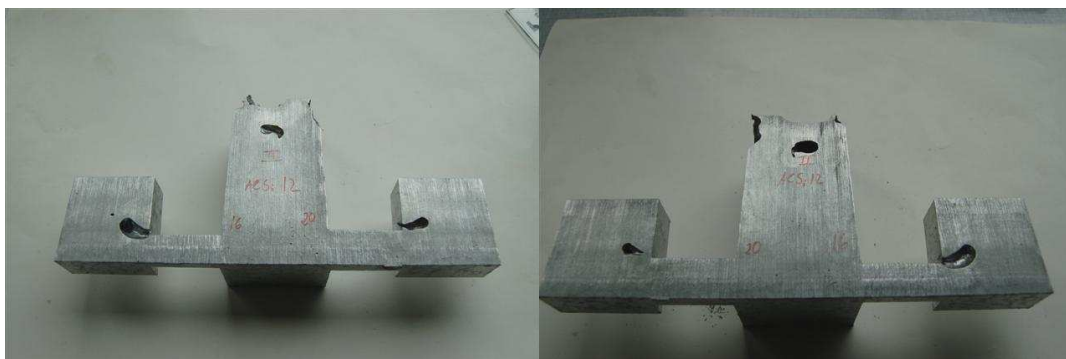


Figure 5.8: AlSi12, short freezing alloy, 16 and 20 mm sections, test II

Figure 5.9 and Figure 5.10a) show detail views of section with 18mm size, obtained in test I and test II respectively. These views are intended to clarify the nature of the defects, since it isn't immediately observable that the defects are surface connected porosities. Figure 5.10b) as the same propose in this case for the 14mm section.

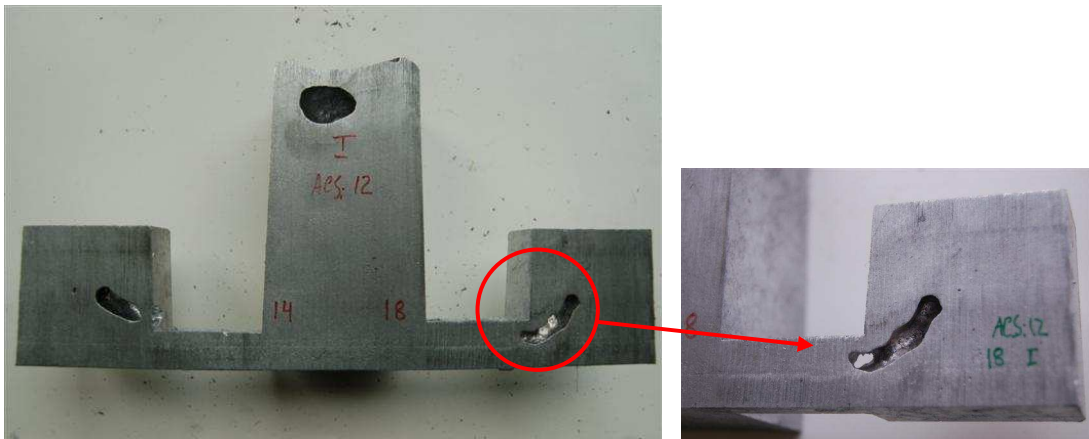


Figure 5.9: Detail view from section 18mm, test I (shows a surface connected defect).

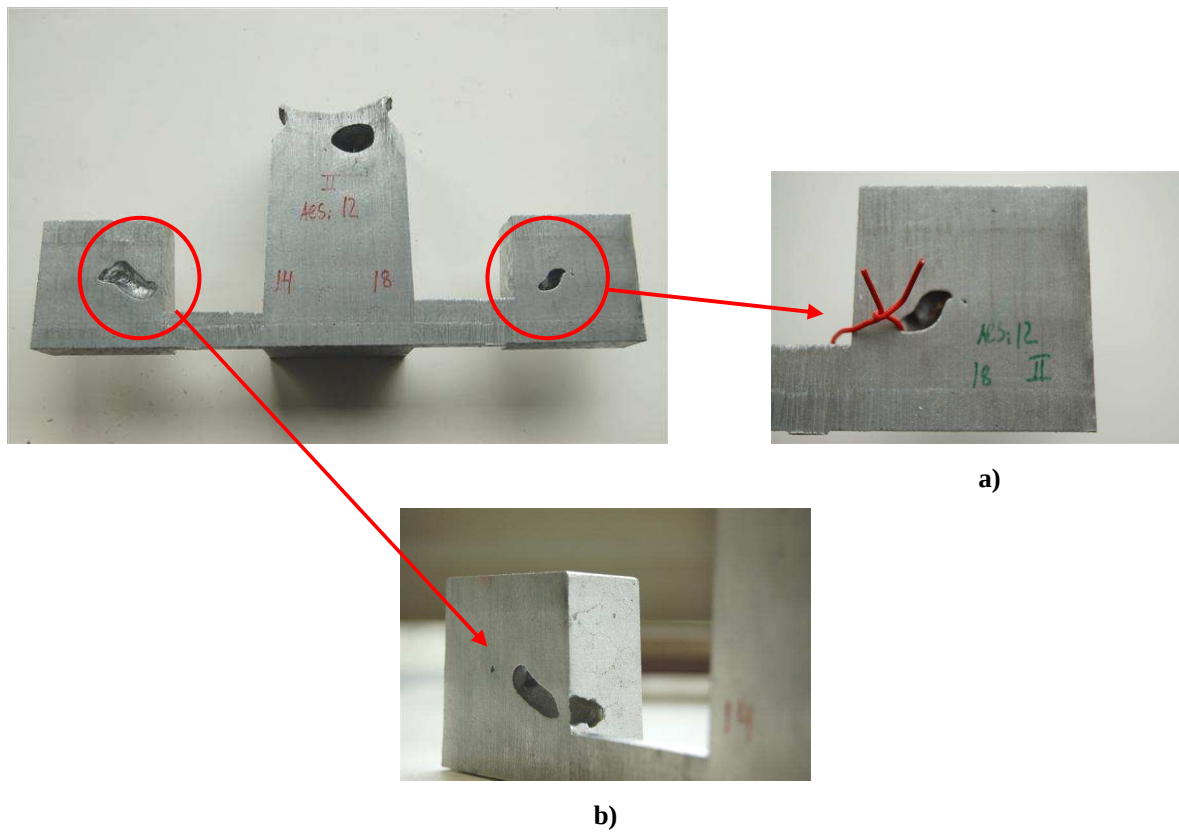


Figure 5.10: Detail view from section a) 18mm and b) 14 mm, test II, showing that the porosity found is surface connected.

5.3.2. AlSi7

In this section results for the long freezing alloy, AlSi7 are presented.

5.3.2.1. AlSi7, sections 14 and 18 mm

Figure 5.11 and Figure 5.12 present the central saw cut B-B, for the two castings, test I and II respectively (poured at same time) AlSi7.

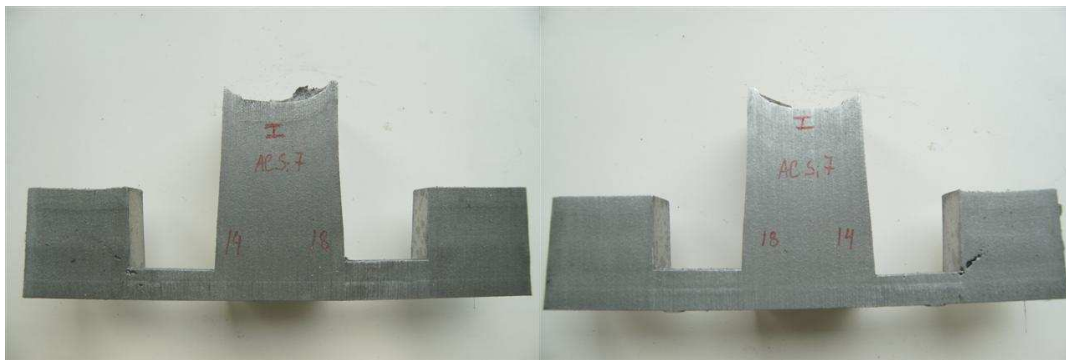


Figure 5.11: AlSi7, long freezing alloy, 14 and 18 mm sections, test I.

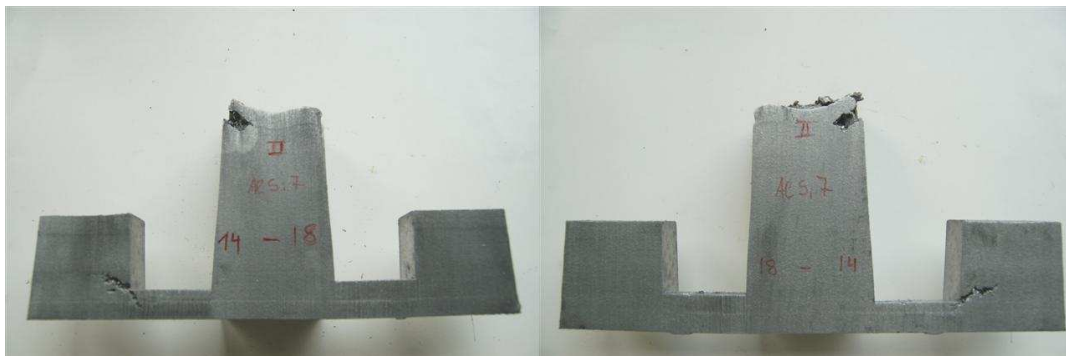


Figure 5.12: AlSi7, long freezing alloy, 14 and 18 mm sections, test II.

5.3.2.2. AlSi7, sections 16 and 20mm

Figure 5.13 and Figure 5.14 present the central saw cut A-A, for the two castings, test I and II respectively.

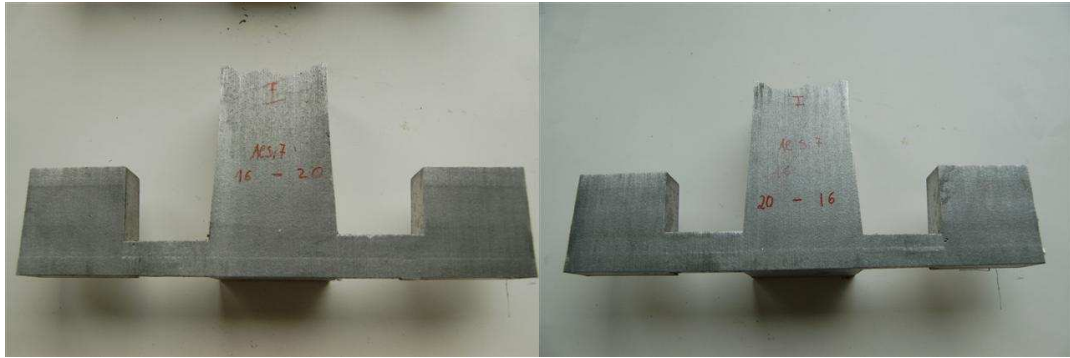


Figure 5.13: AlSi7, long freezing alloy, 16 and 20 mm sections, test I.

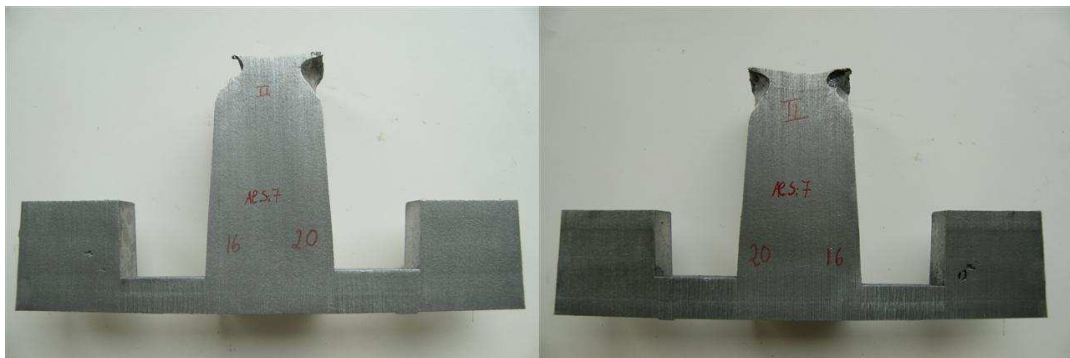


Figure 5.14: AlSi7, long freezing alloy, 16 and 20 mm sections, test II.

Figure 5.15a) shows a top view of the neck with 14mm, showing the surface sink. This defect is also shown in detail view in Figure 5.15b) together with the surface connected defect found in the re-entrant angle.

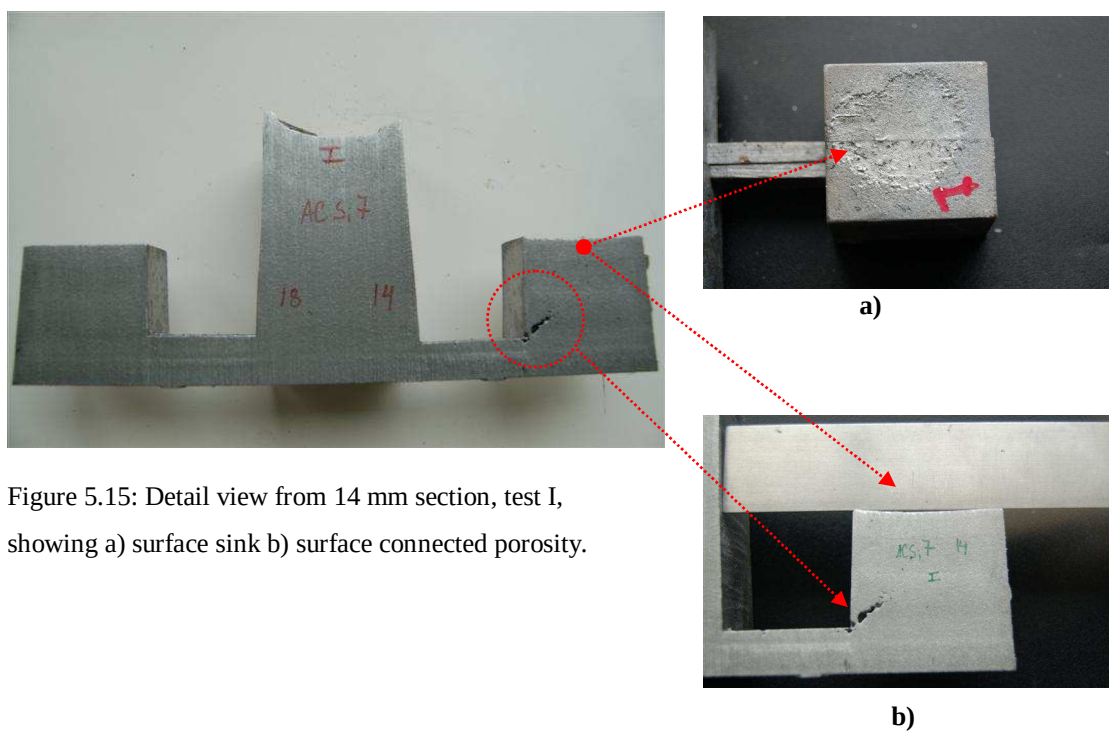


Figure 5.15: Detail view from 14 mm section, test I, showing a) surface sink b) surface connected porosity.

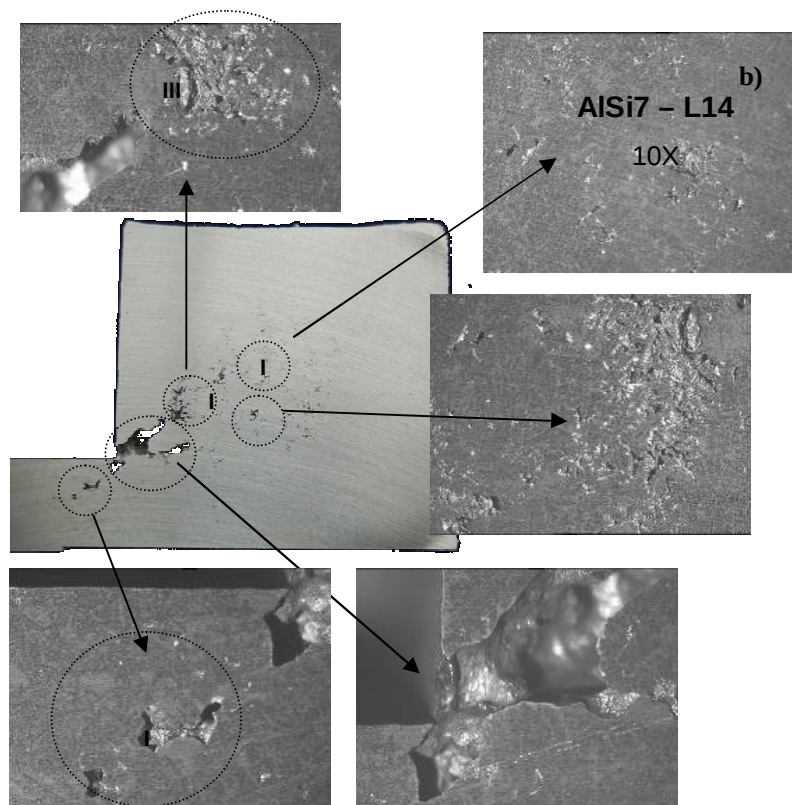


Figure 5.16: Detailed view of surface connected porosity found in AlSi7 with smaller neck, L=14mm.

Long-freezing-range alloys will be filled with a mesh of dendrites in a sea of residual liquid. In this case liquid feeding effectively becomes interdendritic feeding. As the liquid drains out to feed more distant regions of the casting (path becomes obstructed), air will be sucked in, in order to replace it. When sectioned, the porosity resembles a mass of separate pores in regions separated by dendrites, as shown in Figure 5.16. It is therefore often mistaken for isolated interdendritic porosity.

Key points

The main defect found in AlSi12, short freezing, is surface connected porosity, that decreases as the neck section (feeding path) increases from 14 to 20mm. Noticeable external sinks where absent.

In AlSi7, long freezing, a sink in the top of the part, and an inner shrinkage porosity are observed (also more critical in the 14 mm section).

5.4 Simulation conditions

5.4.1. Geometrical data

To adequately represent the geometry, a finite-volume mesh of 231.770 total elements was used. 19.330 were metal elements and 212.440 were sand elements.

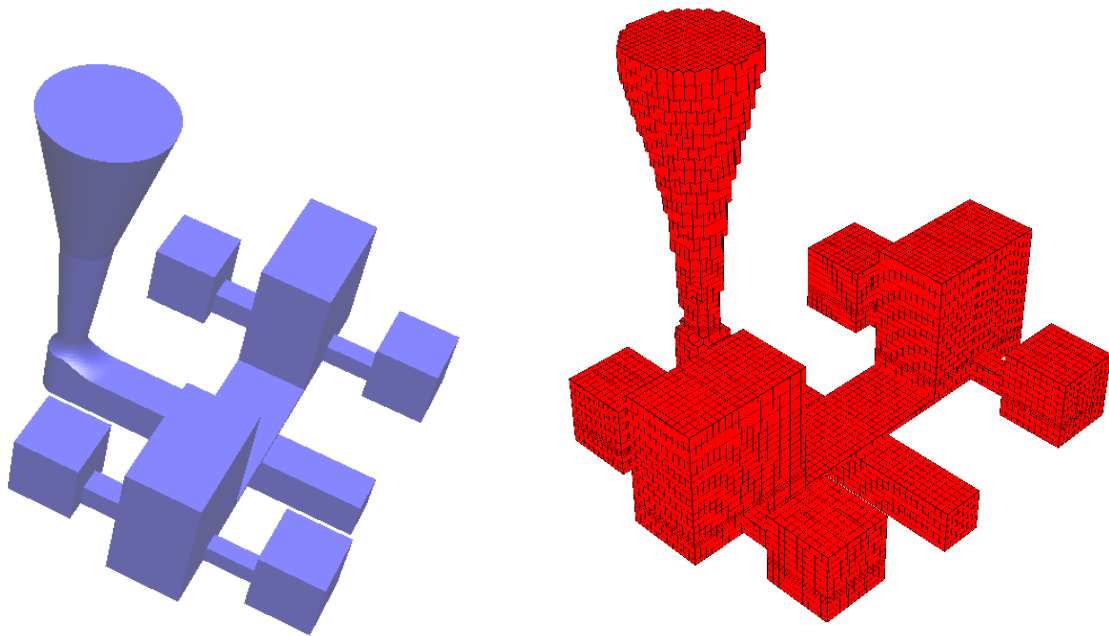


Figure 5.17: 3-D geometrical model and mesh of finite volume.

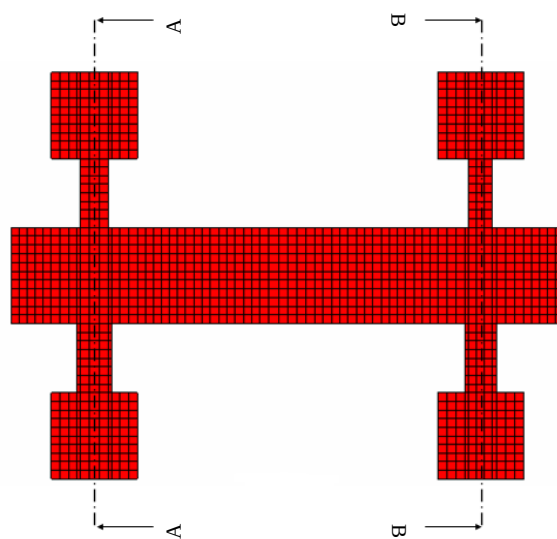


Figure 5.18: Top view. Location of cuts, shown in Figure 5.19.

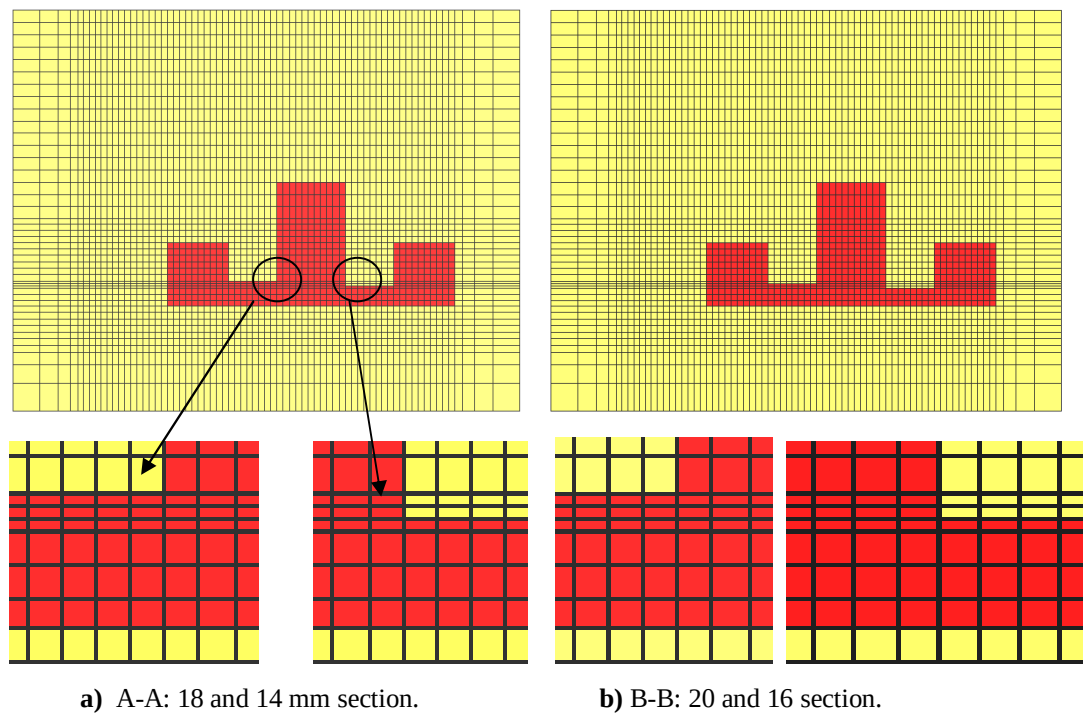


Figure 5.19: Cut sections (Figure 5.18).

The numerical parameters used in discretisation are presented in Table 5.1. Table 5.2 presents the number of time steps and CPU time needed for each material.

Table 5.1: numerical parameters

	dx	dy	dz	n° of elements	Time step
metal	3-4mm			19330	0.001s
sand	5-30mm			212240	

Table 5.2: Number of time steps and CPU time

	n° time steps	CPU time
AlSi12	621304	201600
AlSi7	860264	331200

The model parameters used can be found in 2.4.6.

5.5 Numerical results and comparison with experiments

5.5.1. AlSi7 – Long freezing alloy

In a long freezing material the free surface will be able to feed the casting much longer and eventually most of the shrinkage will be compensated by the movement of the outside surface. When the connecting section is solidifying, the path between the feeder and the part becomes obstructed resulting in a pressure drop in the part. Initially, sinking of the top surface is observed, Figure 5.21a) resulting in a sloped top surface, Figure 5.20. Eventually the top surface will be solidified and feeding from this surface stops. Pressure will continue dropping until any other surface element equals the outside pressure. By then, if these elements are still liquid enough, they can freely move to compensate shrinkage as shown in Figure 5.21b) (re-entrant angle elements).

5.5.1.1. AlSi7 – 14 mm section

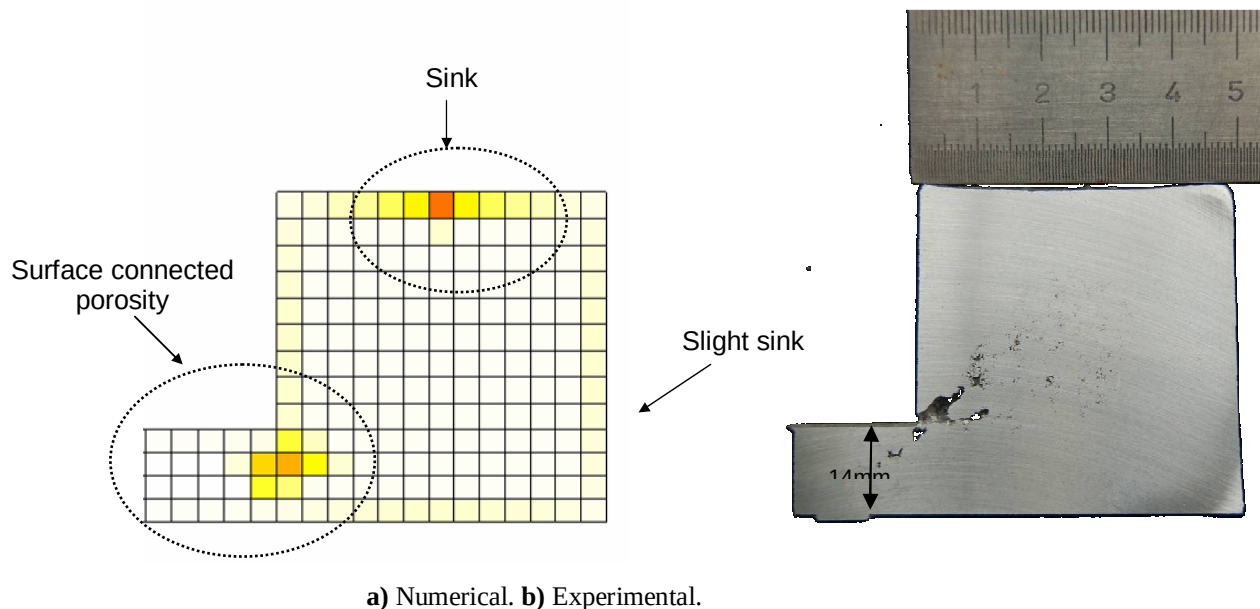


Figure 5.20: Shrinkage defects distribution, AlSi7 L=14mm.

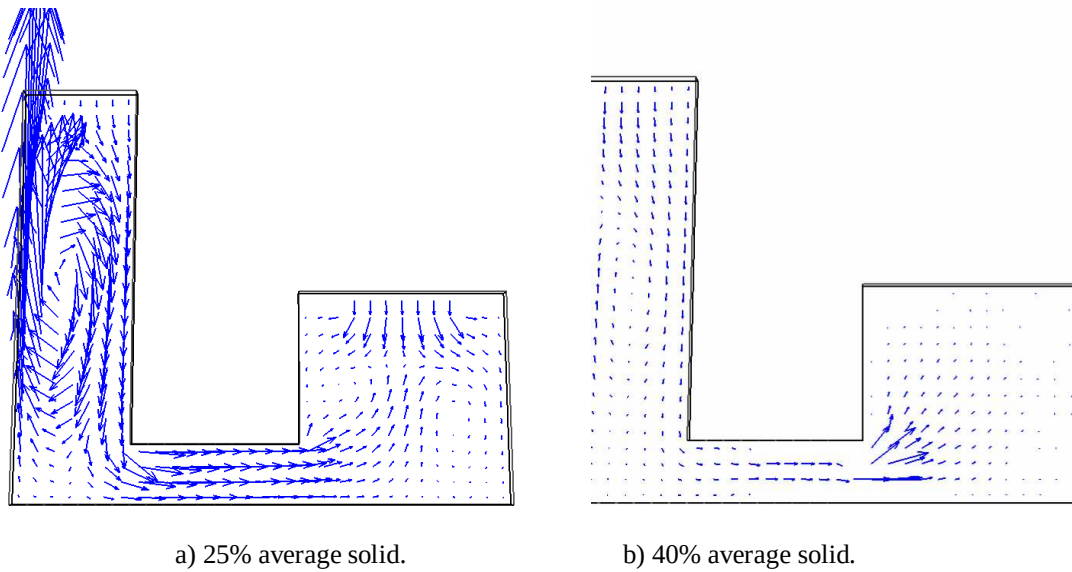
Shrinkage mechanisms:

Figure 5.21: Feeding velocity field.

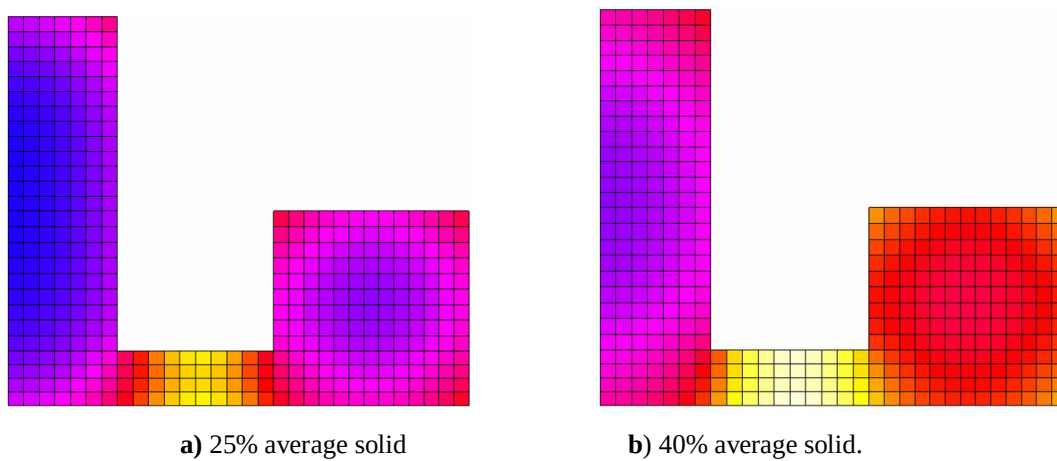


Figure 5.22: Solid fraction.

Figure 5.22 presents the solid fraction distribution when the feeding mechanisms are activated, top feeding at 25%, Figure 5.22a), and feeding from re-entrant-angle at 40% average solid, Figure 5.22b).

Figure 5.24 shows the solid fraction evolution for three locations pointed in Figure 5.23. As expected, due to a mushy solidification, characteristic of long freezing materials, a very similar behaviour for the three different locations was found.

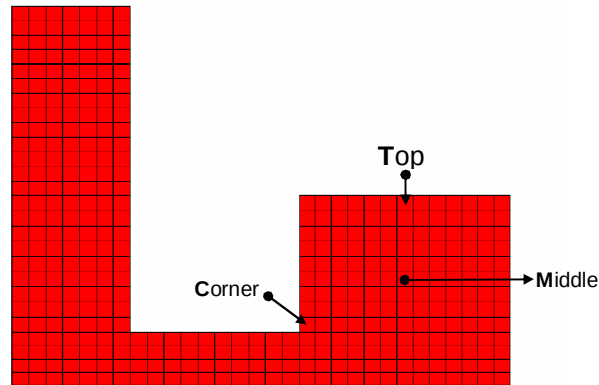


Figure 5.23: Location of control points, a **Top** element, a **Middle** element and a **Corner** element.

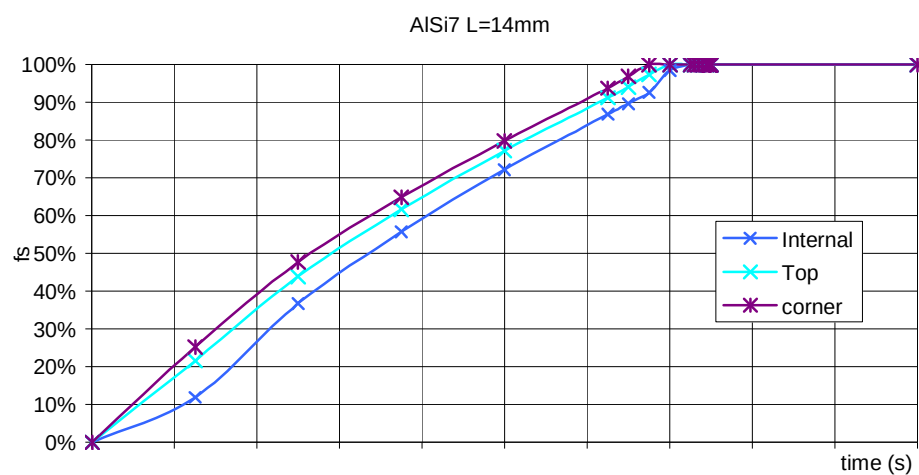


Figure 5.24: Solid fraction evolution.

In Figure 5.25 the cooling curves for the same points are presented.

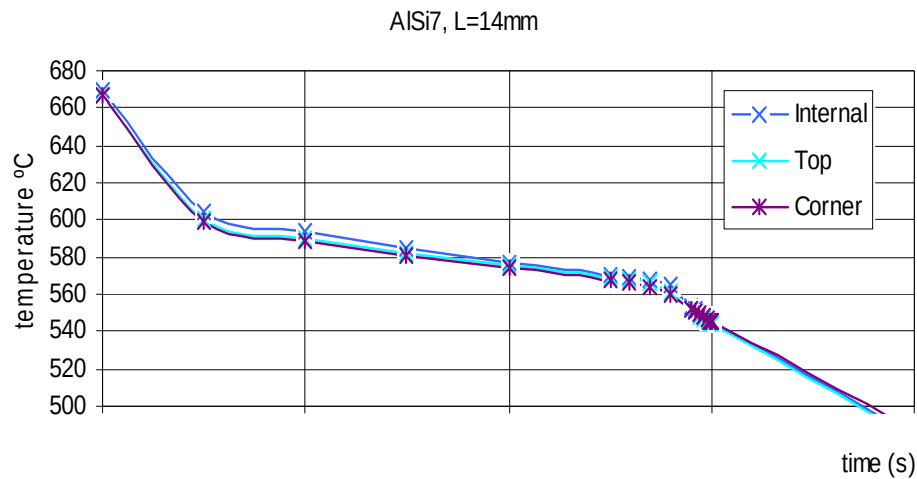


Figure 5.25: cooling curves.

In Figure 5.26 the pressure evolution for the three locations is presented. When the connecting is solidifying, the path between the feeder and the part becomes obstructed resulting in a pressure drop in the part. The top surface element is the first to reach the atmospheric pressure, after which it will be able to feed the part. Mid time the pressure will continue to drop inside the casting, and eventually the corner surface element also reaches the outside pressure and will start feeding the part releasing the pressure inside the casting, seen by the stabilization of pressure drop in the middle element, Figure 5.27.

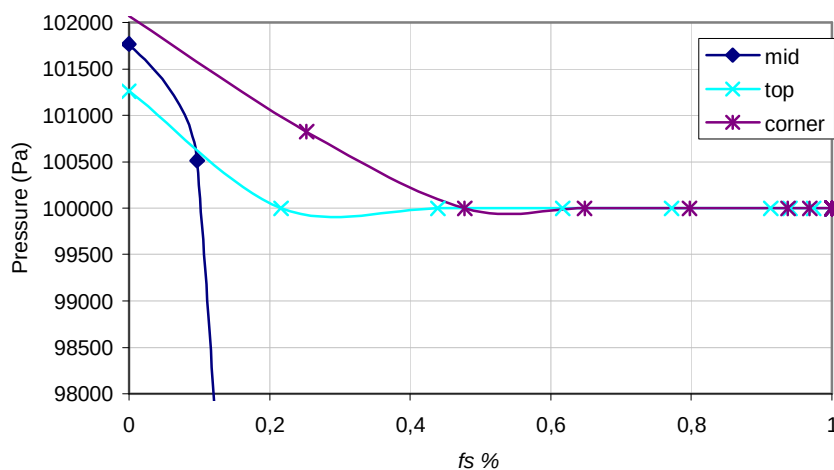


Figure 5.26: Pressure evolution and solid fraction.

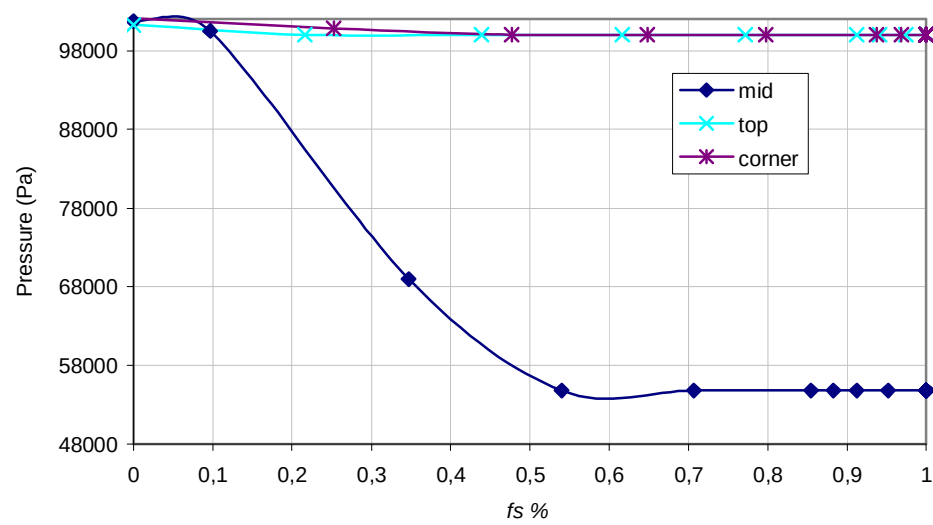
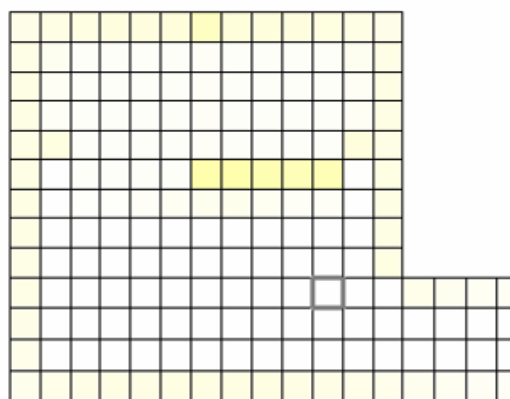
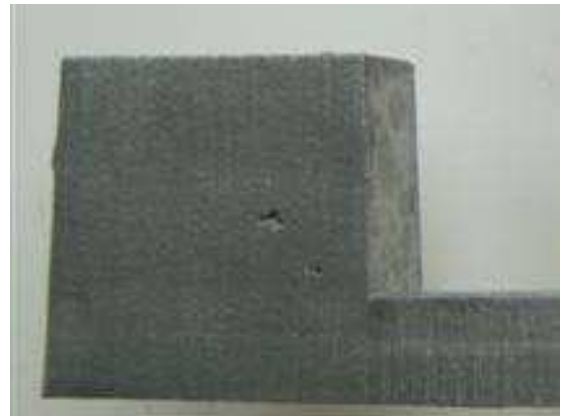


Figure 5.27: Detail of pressure evolution, stabilization of mid point pressure drop.

5.5.1.2. AlSi7 – 16 mm section



a) Numerical.



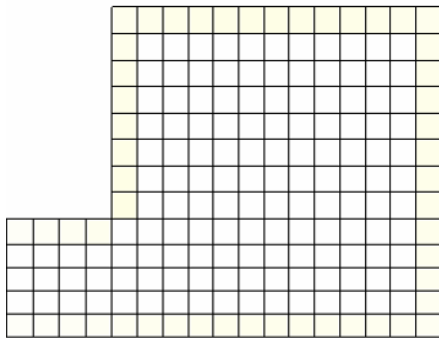
b) Experimental.

Figure 5.28: Shrinkage defects distribution, AlSi7 L=16mm.

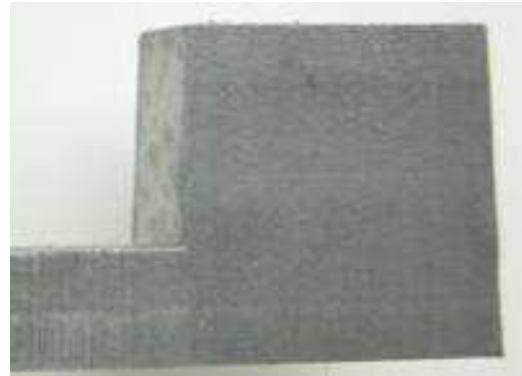
For L=16mm, Figure 5.28 almost no internal porosity is found due to the larger cross section allowing a correct feeding from the feeder.

5.5.1.3. AlSi7 – 18 mm section

As the neck size increases, the amount of defects in the part decreases, and ultimately only a slight sinking is observed for L=18mm.



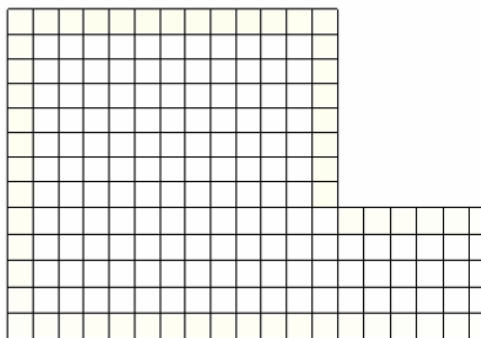
a) Numerical.



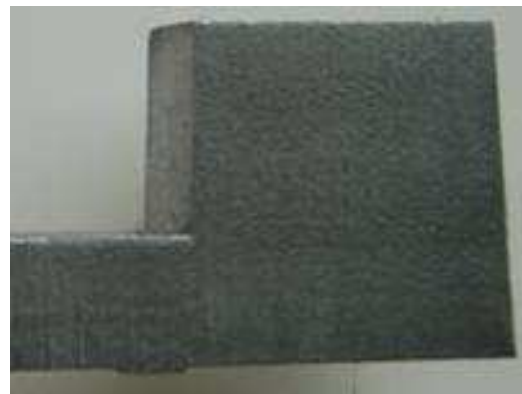
b) Experimental.

Figure 5.29: Shrinkage defects distribution, AlSi7 L=18mm.

5.5.1.4. AlSi7 – 20 mm section



a) Numerical.



b) Experimental.

Figure 5.30: Shrinkage defects distribution, AlSi7 L=20mm.

The part with 20 mm connecting section doesn't present any visible defects.

5.5.2. AlSi12 – Short freezing alloy

When considering a short freezing material, the outside layer quickly solidifies and it is difficult to feed through a free surface movement. Due to shrinking, the pressure in the inner part quickly drops resulting in internal, or surface connected shrinkage porosity, as seen in Figure 5.31 a) numerical and b) experimental.

5.5.2.1. AlSi2 – 14 mm section

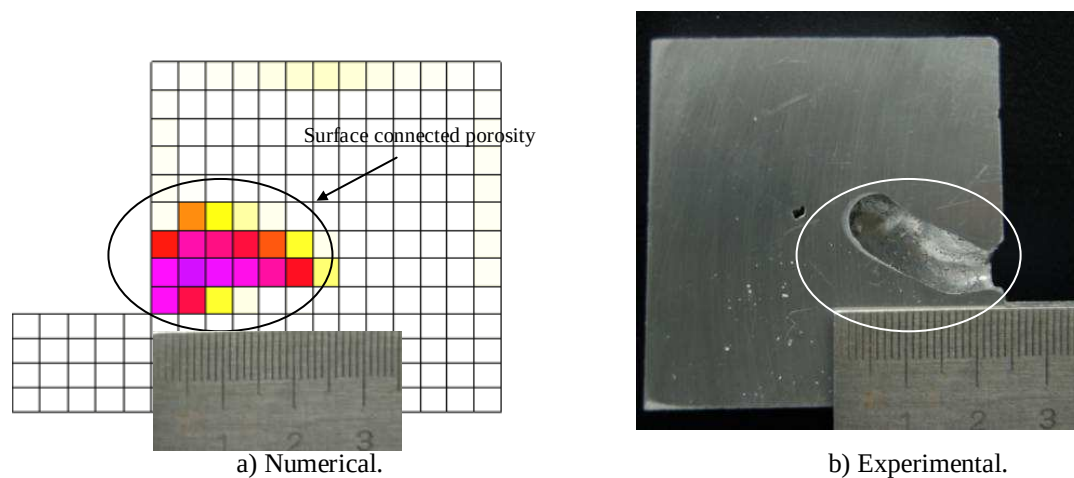


Figure 5.31: Shrinkage defects distribution, AlSi12, L=14mm.

In Figure 5.32 the cooling curves for the same points are presented as in Figure 5.23.

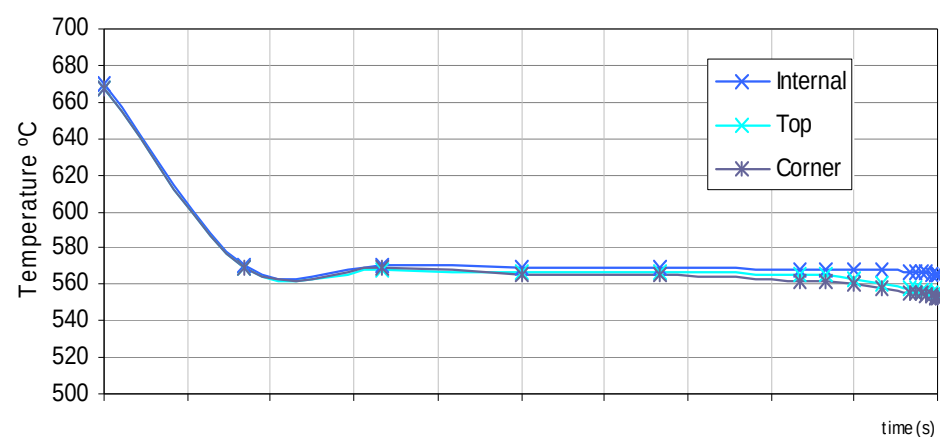


Figure 5.32: Cooling curves numerical measurements at locations pointed in Figure 5.23.

Figure 5.33 shows the solid fraction evolution for the same three locations. As expected, due to the skin freezing characteristic of short freezing materials, the three locations present a

very different behaviour opposite to what happened with the long freezing alloy AlSi7. Solidifying much more quickly in the outside layers, top and corner than in the middle. The speeding up in the solidification of the corner element is justified by the air being drawn in.

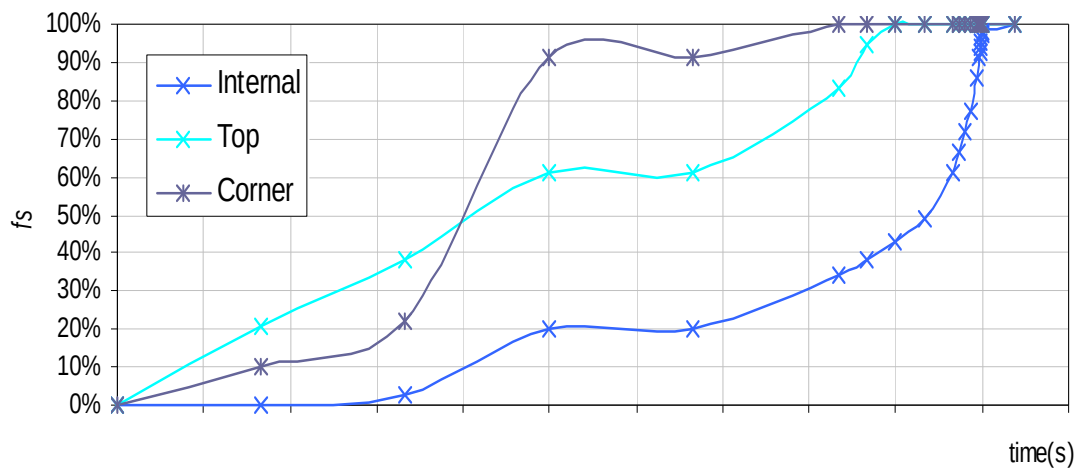


Figure 5.33: Solid fraction evolution.

The first location to reach atmospheric pressure is the corner element, Figure 5.34, has a low solid fraction, which means that this location is liquid enough to move and to feed the part. Only later on, the pressure will drop in the top surface to reach the atmospheric pressure, but, at this moment the outside layer has already highly solidified and feeding from here is very difficult. Inside the casting the pressure is released as soon as feeding from the surface corner starts, Figure 5.34.

AlSi12-L14mm

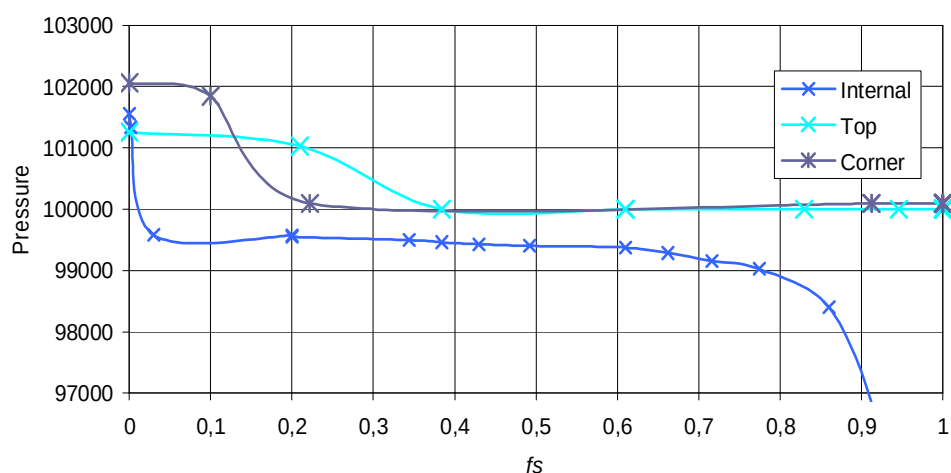
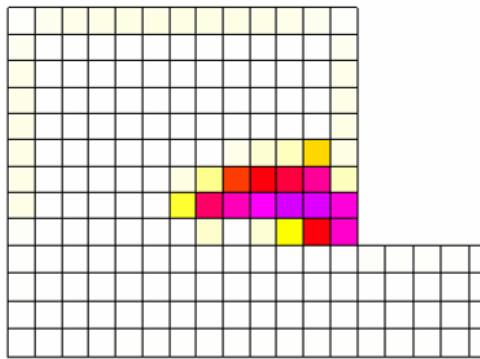


Figure 5.34: Pressure evolution and solid fraction.

5.5.2.2. AlSi12 – 16 mm section



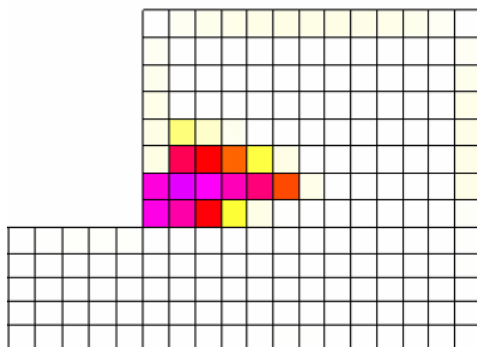
a) Numerical.



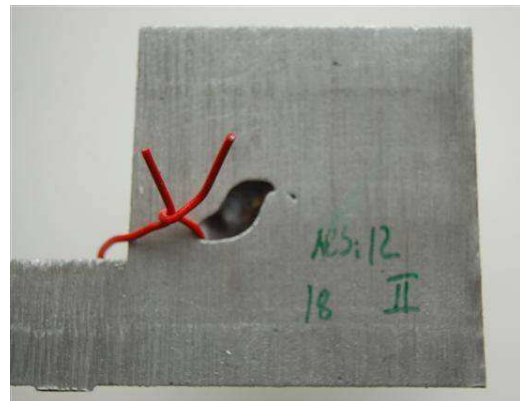
b) Experimental.

Figure 5.35: Shrinkage defects distribution, AlSi12, L=16mm.

5.5.2.3. *ALS12 – 18 mm section*



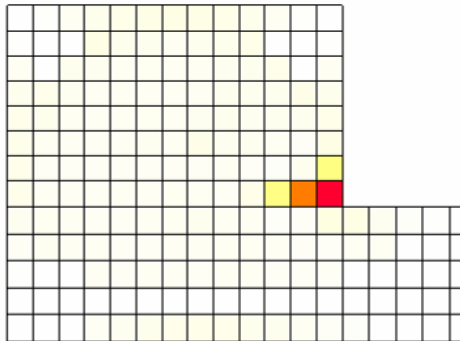
a) Numerical.



b) Experimental.

Figure 5.36: Shrinkage defects distribution, AlSi12, L=18mm.

5.5.2.4. AlSi12 – 20 mm section



a) Numerical.



b) Experimental.

Figure 5.37: Shrinkage defects distribution, AlSi12, L=20mm.

As the neck size increases the severity of the defect is attenuated, though the larger section L=20mm still presents a significant inside defect, Figure 5.37.

Key point

When considering a short freezing material, the outside layer quickly solidifies and it is difficult to feed through a free surface movement. Due to shrinking, the pressure in the inner part quickly drops resulting in more internal shrinkage porosity. However, in a long freezing material the free surface will be able to feed the casting much longer and eventually most of the shrinkage will be compensated by the movement of the outside surface. This is in correspondence with the general observation.

5.6 Volume of shrinkage

5.6.1. Volume of defects

As expected the “worst” results in terms of volume of defects were found for the smaller cross section size, 14mm. In the AlSi12 alloy, since it has skin solidification, surface sinks weren’t as severe as in the AlSi7. Instead, the main defects found were surface connected porosity.

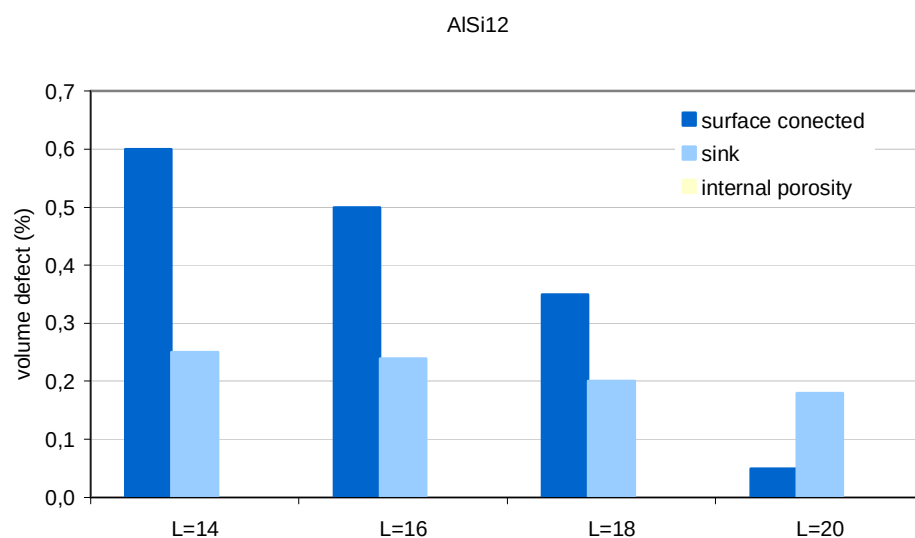


Figure 5.38: Amount of defects (volume pct) found in each section in AlSi12.

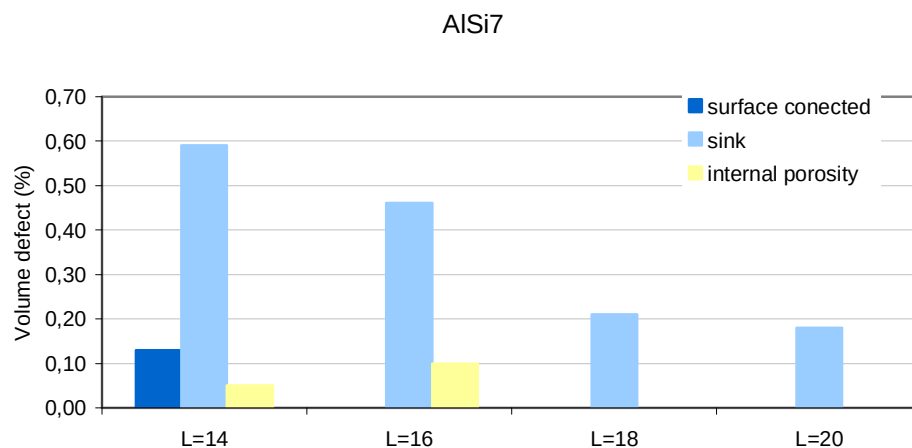


Figure 5.39: Amount of defects (volume pct) found in each section in AlSi7.

5.6.2. Distribution by type of defect

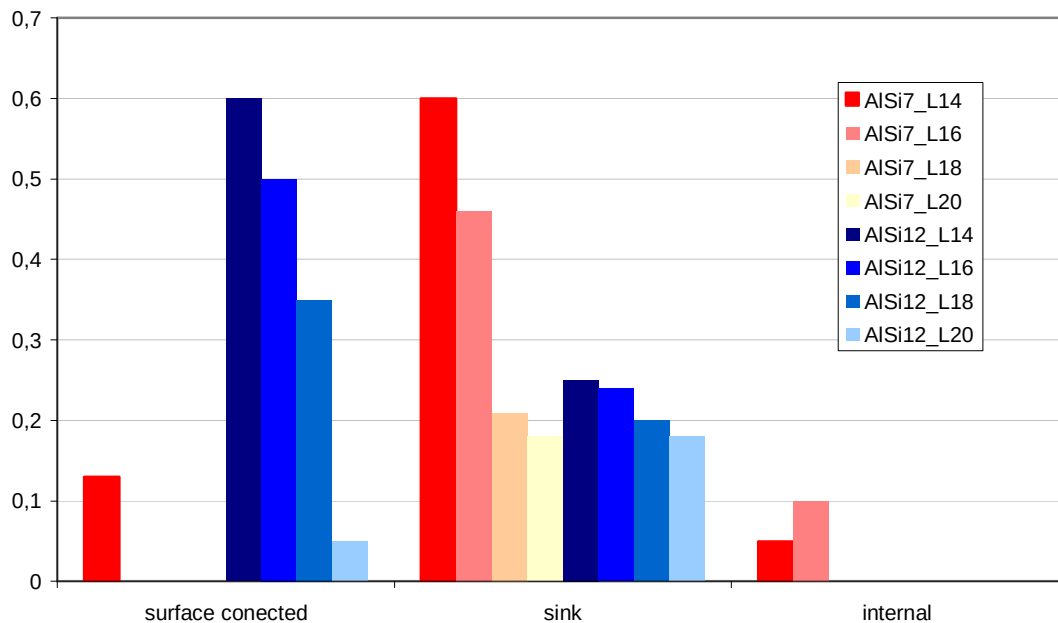


Figure 5.40: Defects distribution, surface connected sinks and internal porosity.

Although the total shrinkage is almost identical, the freezing range is found to have a pronounced effect on the internal or external distribution of porosity. The short freezing range alloy exhibits mainly internal shrinkage that is surface connected, whereas the long freezing range alloy exhibits mainly external porosity in the form of sinks.

Key point

The location and severity of shrinkage defects predicted by other methodologies are based on thermal/volume analysis and therefore, they don't have the ability to predict regions, where interdendritic cavity or surface sinks defects form.

The current developed model uses an approach based on the feeding deficiencies phenomenon in order to accurately localize and quantify shrinkages defects. The results showed the capability of the "defect" model to predict the shrinkage defects. The model gives the correct trend in predicting the location, extent, and nature of the shrinkage porosity defects.

CHAPTER 6

CONCLUDING REMARKS

*Comments on the success and failure of the aims and objectives of this thesis are presented.
Any problems that have arisen are discussed and recommendations are provided for future
work.*

6.1 Conclusions

The process modelling of shape casting is geometrically complex and computationally very challenging. Besides the three-dimensional complex shapes with multiple domains, the defects of interest to industry arise as a consequence of the interaction amongst a range of phenomena. Conventionally, the key phenomena and defect prediction are modelled through empirical relations applied to the simulation results. Such approaches are neither comprehensive nor reliable.

This thesis presents a 3-D model that is capable of predicting the formation of shrinkage defects explicitly as a function of the interacting continuum phenomena i.e. free surface flow, heat transfer, and solidification, in complex three-dimensional geometries. The developed physics-based model for shrinkage defects intends to capture the different behaviour in solidification of skin freezing material and mushy freezing alloy by predicting location and extent of internal and external shrinkage.

6.1.1. Proposed model

This thesis presents a 3-D model that is capable of predicting the formation of shrinkage defects explicitly as a function of the **interacting continuum phenomena** i.e. free surface flow, heat transfer and solidification, in complex three-dimensional geometries. The aim of the physics-based developed model was to capture the different behaviour in solidification of **skin freezing** and **mushy freezing** alloy by predicting location and extent of internal and external shrinkage.

This model and corresponding validations have been applied to AlSi alloys. In this model different types of defects can be predicted: porosity by surface initiation, external porosity and internal porosity by nucleation.

a) Internal porosity by surface initiation

To model surface connected defects, the present approach considers that when there is insufficient pressure inside the casting, the liquid which is still connected to the outside

surface may be drawn from the surface, causing the growth of porosity which is connected to the surface.

This type of defect was found in both short and long freezing alloys, although having different appearance. In the long freezing alloy AlSi7, what seems to be a series of separate interdendritic pores, is in reality a single interconnected pore with a highly complex shape. On the other hand, the short freezing alloy AlSi12 reveals a single and evident cavity.

Numerical results showed that in the long-freezing-range alloy this type of defect occurred at a late stage in solidification, when developing the dendritic mesh (higher solid fraction-less permeability). This means that drawing liquid from the nearby surface becomes easier than drawing liquid from the more distant feeder. The point from which liquid may be drawn can be any surface and a random point in a surface. However, in the short freezing alloy, the initiation site begins at the surface and is much more localized.

b) Internal porosity by nucleation

The short-freezing-range alloy forms a sound and solid skin at the early stages of freezing, while liquid feeding is still possible through wide open channels. When this path is blocked, any final lowering of the internal pressure (here it was concluded that the specific value of the critical pressure isn't significant), due to poor feeding towards the end of freezing, may then create a pore by nucleation in the interior liquid. In this case there is clearly no connection with the outside surface of the casting. After nucleation, further solidification will provide the driving force for growth of the pore. Once the pore is formed, the internal stress will be eliminated and further solid feeding is stopped. The action of the remaining solidification shrinkage is simply to grow the pore. In the situation where the shrinkage problem is in an isolated central region of the casting, in a narrow-freezing-range material any resulting shrinkage pore will again be a smooth single cavity.

c) External porosity

Surface sink (top and side) were found in long freezing alloys. They were particularly evident when the path from the feeder was smaller. This means that the lowering in internal

pressure happened very soon and lead to an inward movement of the external surface of the casting, since it wasn't solid enough to resist the pulling due to pressure drop. If the movement is severe and localized it constitutes a defect known as a 'sink' or a 'draw'. The external movement of the casting will occur before the internal pressure falls to the level required to nucleate an internal pore.

6.1.2. Model validation

Several test cases of increasing complexity are presented. Two aluminium–silicon alloys, a short freezing and a long freezing alloy were studied. Three case studies are presented. The first case purpose was to test the ability of the model to capture different behaviour of alloys with different freezing ranges. The second test case has been used as a first validation of the model by experimental comparison. Finally, a third test case with a 3-D complex shape has been also used for validation purposes by comparing numerical and experimental results.

a) First test case -“Box test”

The **first test case** was a simple 3-D geometry, a square “Box”, presented in chapter 4. A number of theoretical simulations were performed in order to observe the features of the developed model. The aim of these tests was to test the sensitivity of the model in capturing different behaviour of alloys with different freezing ranges.

Results revealed, as expected, that in the short freezing material the outside surface layers quickly solidified. Therefore the movement of the outside layers in order to compensate the volume deficit due to shrinkage ended very soon. Then the pressure quickly dropped and the criterion to form a pore was met. This observation already showed that, probably, the critical pressure criteria wouldn't influence the results because when the pressure starts to drop, if no other feeding mechanism is activated, inevitably the critical pressure is reached.

It was observed that as long as the outside layers compensate the volume deficit by solidification, the feeding velocity was directed from the surface to the inside, *i.e.* the metal was driven by the pressure gradient from the outside to the inside. As soon as a pore was formed the feeding velocity was directed away from the pore to the outside, because the pressure inside the pore was higher than the pressure of the surrounding liquid, which was shrinking. This resulted in a sudden direction change of the velocities when a pore opens. As a result, the movement of the surface to the inside immediately stopped.

In the long freezing material the outside layers remained mushy for a longer time and were able to compensate shrinkage by their significant movement. This resulted in less shrinkage

porosities formed in the inside of the casting, because most of the shrinkage was already compensated by the movement of the outside layers.

The results of the model showed that pore formation occurs earlier in short freezing range alloys than in long freezing range alloys. As a consequence, more internal shrinkage porosities were developed in short freezing alloys than long freezing alloys, because more volume deficit due to shrinkage has to be fed from the pores. The difference found in the top surface shape was also very clear. The short freezing material presented a pronounced depth, whereas the long freezing material showed a much flatter surface.

Though the total amount of shrinkage is identical, the freezing range was found to have a pronounced effect on the internal or external distribution of porosity. The long freezing range alloy exhibited mainly external porosity and a distributed small internal porosity, whereas the short freezing range alloy exhibited mainly concentrated internal shrinkage, i.e. one large hole, porosity and a much sharper top shape.

Qualitatively, the calculations resembled differences between short and long freezing alloys as found in actual castings. One may conclude that the presented numerical model could describe depression of the surface during solidification, as well as the formation of shrinkage porosities.

b) Second test case- “cup test”

The second test case, the cup test presented in chapter 4, allowed exploring the effect of parameters and boundary conditions in the model.

The key parameters for the shrinkage porosity model are the permeability coefficient K_0 , which characterizes the flow resistance during solidification and the porosity initiation pressure, P_{crit} , below which voids are assumed to nucleate within the liquid phase.

A parametric variation of these quantities was performed in a three dimensional simple shape. The influence of the freezing interval, columnar or equiaxed solidification and mesh size was also analyzed.

These tests allowed identification of a parametric range for the permeability coefficient constant, K_0 . The proposed model considers that K_0 is set to two different values during solidification, one value before and another one after coherency.

Before coherency a higher permeability is considered, since the feeding flow can't actually be considered interdendritic. The value assumed was found in the literature and experimentally validated for this type of alloys (AlSi). The performed tests were linked to the value that K_0 should assume after coherency. Three possibilities were tested: maintaining the same permeability coefficient, increasing ten times and increasing one hundred times.

Results from short freezing alloy showed that the upper surface profile presented a deep slope in the centre, which decreases as the permeability coefficient decreases. For higher permeability coefficient the shrinkage defects are concentrated in the form of pipe shrinkage. When increasing K_0 , the pipe shrinkage decreases which is compensated by an increase of the other defects, such as sinks and internal voids.

In the long freezing alloy the upper surface profile doesn't show a significant slope in the centre, as previously found in the short freezing AlSi12, but shows a much more uniform surface. Still the tendency of the decreasing amount of pipe with permeability is also found. As well, the wall defects and internal porosity increases as K_0 decreases.

It was clear that permeability had a significant influence on the macroporosity/voidage formation as might be expected. For a high permeability, the metal can flow to feed the solidifying areas sufficiently well to avoid the deep in the upper level, or as in the long freezing alloy to avoid the shrinkage in the form of sinking of the walls. However, for low permeability, the feeding flow from the upper level is severely restricted resulting in a more profound deep in the top for the AlSi12 short freezing. In AlSi7 long freezing this is revealed in sinking of the wall.

The influence of solidification interval was tested and compared. Again the results showed the ability of the model to represent the differences found in the two types of alloys. These results show that the difference in the top surface shape is clear. The short freezing material presents a pronounced depth, whereas the long freezing material shows a much flatter

surface. As already stated, in a long freezing material the outside layers remain mushy for a longer time and they are able to compensate shrinkage by sink of the surfaces. This results in less shrinkage porosities, formed in the inside of the casting, since the greater part of the shrinkage is already compensated by movement of the outside layers. In the short freezing material the outside layers quickly solidify. Therefore, the volume deficit of the shrinking material is compensated by voids openings.

Different boundary conditions were tested. The aim here was to introduce a condition at the wall boundary, considering that the solidification would be columnar and therefore a smaller value for permeability should be used.

The boundary condition considered for free surfaces was tested. This boundary condition consisted in the assumption that for $f_s > 0.3$ for free surfaces and after coherency, the permeability coefficient was lower in perpendicular direction. Different scenarios were considered for the boundary conditions. The first situation assumed a constant permeability coefficient through the whole solidification, i.e. no special boundary condition. In the second scenario a ten times smaller value for K_0 is considered at the surface after solid fraction exceeded the coherency fraction. In the third situation a one hundred times smaller value was taken.

As expected, the previous boundary condition had a clear influence on the results. When no condition is set, the slop in the top is less pronounced and the shrinkage is compensated by depression of other free surfaces, resulting in sink defects. This is explained by the free surfaces keeping the ability to feed shrinkage throughout the whole solidification period. If this condition is introduced, the ability to feed shrinkage through the free surface decreases.

Several critical pressures, P_{crit} , that could be used in complex shape casting simulations were tested. Results showed that the impact of initiation the pressure was very small. It was clear that once the pressure started to decrease and no other feeding mechanism was activated, the initiation pressure inevitably reached a certain level for a pore to nucleate. The simulation results confirmed that the model was insensitive to this parameter.

The experimental results were compared with different numerical results. From comparison, it became quickly visible which appropriate parameter range of permeability coefficients would adequately reflect the main experimental observations. For solidification after coherency the ten time higher value (when compared to the value used before coherency) was found to give the best results. Considering the boundary at the wall, the best fitting was found when considering a one hundred times higher value compared with the equiaxed solidification.

Another important remark was that unexpectedly the best sets of values were the same for long and short freezing alloys. The reason should be related to the fact that the transition between equiaxed and columnar solidification is very similar for both alloys, due to its minor dependence on silicon percentage.

c) Third test case – “complex shape”

A 3-D geometry with a complex shape and a large number of cells was designed and performed numerically and experimentally, as presented in chapter 5. When designing this geometry the idea was to reproduce a real casting condition, part and feeding system, while maintaining the geometry as simple as possible to better identify the variables directly enrolled in feeding shrinkage. Another requirement has been obtaining geometry prone to different types of shrinkage defects as to illustrate the features of the developed model. This “3-D complex casting”, was composed by a feeding system and blocks with different section sizes.

Two pieces were cast at the same time for each alloy. Important evidence was the repeatability in the two pieces, thus allowing a good confidence in results.

The results showed internal and outside shrinkage defects depending on the freezing range of the metal. As expected, due to freezing characteristics, the short freezing material AlSi12 and the long freezing AlSi7 presented a very different behaviour. In the short freezing alloy the surface connected porosity was much more visible and concentrated in a single cavity while in the long freezing alloy the surface connected porosity had a much more complex shape in the form of an interdendritic cavity. Other clear evidence was the surface sinking that was mainly visible in the long freezing material. It was important to clarify the nature of the

defects, since the nature of the defects found in the long freezing alloy was not immediately evident. When sectioned, the porosity resembled a mass of separate pores in zones separated by dendrites, and therefore could be mistaken for isolated interdendritic porosities instead of for a single cavity.

As expected for both alloys the “worst” results in terms of volume of defects for both alloys, were found for the smaller section of 14mm size.

The main defect found in the AlSi12 short freezing material was surface connected porosity that decreased as the neck cross section (feeding path) increased from 14 to 20 mm. Noticeable external sinks were absent.

In the AlSi7 long freezing material, a sink in the top of the part and surface connected shrinkage porosity were observed in the 14 mm section. As the section increased, the top sink became imperceptible. Also the interdendritic surface connected cavities were only found in the piece with smaller necks section size, 14 and 16mm.

When considering the **long freezing alloy** an interesting observation was the behaviour of the neck solidification. In the long freezing alloy, due to the mushy solidification, the neck became more quickly obstructed and the pressure inside the part started to drop earlier (when compared to short freezing alloys). This resulted in the top surfaces reaching the atmospheric pressure, after which was possible to compensate the shrinkage of the casting, resulting in a sinking of the top surface. In the long freezing material, the free surface was able to feed the casting much longer, since it wasn't enough solidified and the greater part of the shrinkage was compensated by the movement of the outside surface. This numerical behaviour was confirmed in the experimental results where the long freezing material presented clear sinks, especially in the narrow neck part. As the top surface solidified, feeding from this surface became difficult. Pressure continued dropping until every other surface element equalled the outside pressure. By then, if these elements were still liquid enough, they could freely move to compensate shrinkage as it happened in the re-incoming angle elements. This was particularly visible for the smaller cross section model, which presented a wide interconnected porosity.

These results looked very similar with the experiments and the fact of being a single porosity was confirmed in the numerical results. As the cross section increases, the amount of defects in the part decreases, and ultimately only a slight sinking is observable for the 18 mm cross section neck. Also, this was reproduced in the numerical results, where no interconnected porosity was found for 18 and 20 mm neck size.

When considering a **short freezing material**, the obstruction of the feeding through the neck occurs later on and consequently the pressure starts to drop at a later time in the solidification. This fact together with the fact that the outside layer quickly solidifies (short freezing material) made it difficult to feed through a free surface movement. Further solidification lead to an increasing obstruction of the neck, the pressure in the inner part quickly dropped, but by then the top surface was already considerably solidified and feeding became very difficult. The only surface element able to feed the casting was the corner element that had a low solid fraction, this meant that this location is liquid enough to move and to feed the part. Since this pore formation occurred earlier in short freezing range alloys than in long freezing range alloys the surface connected porosity was much more visible and concentrated in the single cavity while in the long freezing alloy the surface connected porosity had a much more complex shape in the form of a interdendritic cavity.

The expected shrinkage features were well described by the present model and illustrates the capability of the “defect” model to predict the shrinkage defects of interest to the foundry industry. The model gives the correct trend in predicting the location, extent, and nature of the shrinkage porosity defects.

A very promising feature is the ability to predict the surface sink, often discarded by numerical codes but very important when real parts are being manufactured.

6.2 Future directions

In this work, some interacting phenomena in solidification have been modelled. Further investigation and developments should proceed, namely those related with the characterization of model parameters, as well as additional validations, so that the prediction of shrinkage defects may have quantified its effects by using the model presented. Also, new features can be added to extend the applicability of the model.

As a summary of future developments the following directions of research are suggested:

- **Optimization of parameter determination**

An evident line of work for additional research is the determination of K_0 , a crucial parameter in the developed model. Inverse methods for example, could be used for evaluation and optimization of K_0 .

- **Optimization of numerical model**

Under this thesis the efficiency of the numerical model has not been of major concern. However, if the current model development is to be implemented in a commercial code, its efficiency should be improved.

- **Extension to other aluminium alloys**

The next step of this research should be to investigate the model applicability on the AlCu alloy, which is very often used in casting. One of the important remarks found in this study was the fact that the same K_0 has shown good results for the two different alloys, AlSi7 and AlSi12. This should be explained by the fact that AlSi alloys present a common value for the columnar to equiaxed transition (CET). It will be very important to check what happens to other aluminium alloys, like AlCu, since these alloys present a different CET.

- **Nodular cast iron material**

The presented model was developed for materials that shrink during solidification due to density increase, which is the case for most alloys. An exception is cast iron, which finds lots of applications in industry.

Solidification in cast irons is a complex process, which involves shrinkage and expansion. In a first part of solidification, liquid shrinkage occurs through the liquidus temperature. A phase change takes place at this juncture. A portion of the liquid iron transforms to solid austenite. Eutectic expansion follows the liquidus. The remaining liquid transforms into austenite and graphite. Expansion always occurs during the eutectic transformation and it is very significant. The larger specific volume of graphite compensates the smaller specific volume of austenite so that the specific volume of austenite and graphite in the eutectic structure gets larger than the one of the liquid. As such, shrinkage pores should not be formed. This is valid for flake cast iron but not for nodular cast iron. The reason therefore is the much more compact form (spheres) of the graphite phase, due to a change of the eutectic growth mechanism. Such shrinkage faults can again be possible in ductile cast irons.

Understanding and predicting the shrinkage behaviour of ductile cast iron parts is the most important point for successful foundry operations and it would be of great interest to upgrade the proposed model to account for this different solidification behaviour.

- **Gas porosity models**

There has been sustained research effort in the last decade to characterize the factors that control gas porosity. The length scales of these phenomena are micrometers compared to component dimensions of millimeter-centimeter. Nevertheless, microporosity in castings can have a profound effect upon their mechanical and fatigue properties.

The presented methodology can include hydrogen porosity formation and evolution during solidification. Microporosity formation and growth are due to the local pressure drop in the mushy zone, and the calculation of the local pressure during solidification can be used to identify and predict the conditions for the formation of hydrogen and shrinkage porosity.

- **Implementation into current casting simulation code**

The process of design for both performance and manufacture is becoming an increasing “virtual” activity where simulation software tools are used to predict the physical behaviour. In this context, engineers need to predict defects when manufacturing the component, in order to efficiently optimize product development stage. Defect models such as those described previously can be embedded into commercial codes which will form the basis of “next” generation tools for the life cycle design process.

It would be useful to explore the extent to which this model adequately represents all shrinkage defects phenomena in casting, because it is not so numerically complex to implement and run.

Including advanced shrinkage modelling into FD/FE casting simulations is not only possible and realistic from a computational point of view but also necessary for the accuracy of predictions in order to improve design castings avoiding and mastering the skin and internal shrinkage defects.

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