Thermal Analysis of the Startup Phase for D.C. Casting of an AA5182 Aluminum Ingot

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Abstract

The evolution of temperature and stress during the start-up phase of the direct chill (D.C.) casting process has been studied to determine the factors that make this phase of the process prone to surface crack generation. The analysis was carried out principally using a finite element based heat flow model, but a preliminary thermal stress model was also employed. Key to the study was the experimental measurement of temperature in the region of the cast prone to crack formation and the development of a technique to determine the surface heat fluxes as a function of surface temperature (system boiling curves) in the direct chill water.

An inverse heat transfer methodology was developed to calculate the boiling curves for direct chill water cooling. This method uses as input the data acquired from one embedded thermocouple transiting the water cooling region and involves the application of 1-D and 2-D finite element based heat conduction models in succession. The technique has been verified using hypothetical temperature data obtained from a transient casting simulation conducted with a known heat flux profile. The results of the inverse heat calculations on the industrial data indicate that a variation in surface morphology, occurring during the early stages of casting, influences the shape of the water cooling flux/temperature relations and has a bearing on the amount of heat extracted during startup. The intensity of the direct chill water cooling was found to be enhanced in the "lapped surface morphology" portion of the ingot relative to the remainder of the cast.
Based on the calculated system boiling curves, a FEM simulation of the cast start was undertaken. The thermal analysis was employed to identify conditions that may enhance the potential for surface crack generation. The simulation data, in conjunction with relevant industrial measurements, suggests that a combination of an increase in the solidified shell thickness (defined as the distance of the solidus isotherm from the surface of the ingot parallel to the water contact line), and a high surface temperature gradient in the vicinity of the water contact point, accounts for the high incidence of surface face cracking observed.

A preliminary thermal stress analysis qualitatively supports the association of a peak tensile stress with a peak in surface temperature gradient. Maximum values of both shell thickness and peak surface temperature gradient were observed to occur in the “lapped surface morphology” regime. The peak values in this region of the ingot were attributed to both an increase in the severity of water cooling (as calculated with the inverse heat transfer technique) and an enhancement in heat extracted by the mould. This observation indicates that events occurring in the meniscus region, with particular regard to the development of surface morphology, have a significant impact on subsequent cooling behaviour.
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**Nomenclature**

**Latin Symbols**

- $B_j, B_i^T$: matrix of differential operators
- $C_p$: heat capacity, $J/kg \cdot ^\circ C$
- $C, C_e$: global and elemental heat capacitance matrices
- $D$: elasticity matrix
- $E$: elastic modulus, GPa
- $F_i$: body force vector in direction i, MN
- $f, f^e$: global and elemental force vector
- $H$: enthalpy, $J/kg$
- $h, h_i$: vector of heat transfer coefficient global and nodal, $W/m^2 \cdot ^\circ C$
- $K, K^e$: global and elemental stiffness matrix
- $k_i$: thermal conductivity in direction i, $W/m \cdot ^\circ C$
- $N_i$: row vector for interpolation functions for node i
- $N_j$: column vector of interpolation functions for node j
- $Q$: heat flux per unit volume, $W/m^3$
- $q$: heat flux per unit area, $W/m^2$
- $\rho$: density, $kg/m^3$
- $R_{1-D}$: relaxation factor for temperature difference in 1-dimensional analysis
- $R_{1,2-D}$: relaxation factor for temperature difference in 2-dimensional analysis
- $R_{2,2-D}$: relaxation factor for rate of temperature change in 2-dimensional analysis
- $t$: time, sec
- $\Delta t_i$: time step at time i used in numerical integration, sec
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<td>$T$</td>
<td>temperature</td>
<td>°C</td>
</tr>
<tr>
<td>$T_{amb}$</td>
<td>ambient temperature</td>
<td>°C</td>
</tr>
<tr>
<td>$T^e$</td>
<td>elemental temperature vector</td>
<td>°C</td>
</tr>
<tr>
<td>$T_i$</td>
<td>temperature at node $i$ (Eq. 5.5)</td>
<td>°C</td>
</tr>
<tr>
<td>$T_i$</td>
<td>temperature at time $i$</td>
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<tr>
<td>$U_i$</td>
<td>internal potential energy</td>
<td>Nm</td>
</tr>
<tr>
<td>$u, v, w$</td>
<td>local Cartesian coordinate system</td>
<td></td>
</tr>
<tr>
<td>$u_i, v_i, w_i$</td>
<td>displacements for node $i$ in the $x,y,z$ directions</td>
<td>m</td>
</tr>
<tr>
<td>$V$</td>
<td>volume</td>
<td>m³</td>
</tr>
<tr>
<td>$v(t)$</td>
<td>time dependent casting speed</td>
<td>m/s</td>
</tr>
</tbody>
</table>
$W_i$ weighting coefficients for Gauss Quadrature integration

$x, y, z$ global Cartesian coordinate system

$y(t)$ distance below meniscus (Eq. 6.1) $\text{m}$

$y_j$ axial location in 2-D inverse analysis $\text{m}$

**Greek Symbols**

$\sigma_i$ stress in direction $i$ $\text{MPa}$

$\tau_{ij}$ shear stress normal to $i$ in direction $j$ $\text{MPa}$

$\varepsilon_i, \{\varepsilon\}, \{\varepsilon\}_0$ strain in direction $i$, strain vector and initial strain vector

$\varepsilon_p$ deformation strain

$\varepsilon_T$ thermal strain

$\delta, \{\delta\}, \{\delta\}^e$ displacement, displacement and elemental displacement vector $\text{m}$

**Mathematical Symbols**

$\partial$ differential operator

$\nabla$ divergence
ACKNOWLEDGMENTS

I would like to express my deep appreciation to Dr. S.L. Cockcroft for his input and welcome advice. Financial assistance from NSERC and Alcan Ltd. is gratefully acknowledged. I would also like to thank Erach Tarapore and Norm Walker of Kaiser Aluminum for providing access to the industrial caster.

In conclusion, completing a Ph.D. involves more than solitary study but includes an array of colleagues who always seem to challenge you intellectually and who also make semi-decent canoeing partners. A modified version of Robert Service’s “The Spell of the Yukon” best expresses this idea:

I wanted a Ph.D. and I sought it,
I scrambled and mucked like a slave.
Was it proposals or papers - I fought it;
I hurled my youth into the grave.

I wanted a Ph.D. and I got it,
came out with my degree last fall -
Yet, somehow life isn’t as I thought it
and somehow the thesis isn’t all.
1. Introduction and Background

1.1 Introduction

The D.C. (direct chill) semi-continuous casting process has been the mainstay of the aluminum metal industry for the production of billets and ingots since the 1930s. As the name implies, the defining character of this casting method is the direct contact of the cooling water with the solidifying ingot. A schematic of a cross section of the process is shown in Figure 1.1. The main components of the system include a mechanism for delivering molten metal, a water cooled aluminum mould, the direct chill water jets, a starting block and a moving casting platen. Included in the figure are the metal level in the mould and the typical position of the solid/liquidus interface within the ingot. Casting proceeds by lowering of the platen such that the ingot is continuously withdrawn from the mould where it is rapidly cooled by the direct water jets. The rate of ingot formation (platen drop rate) is balanced by an equivalent flow of molten aluminum into the mould to maintain a constant metal level. An entire casting sequence includes: a start up phase where the initial portion of the ingot is established, a steady state regime defined by a stationary solid/liquid interface relative to a coordinate system fixed with respect to the mould and an ending phase occurring at the point of maximum platen drop below the mould.
For the D.C. casting system described above, heat flows by conduction/convection from the liquid metal to the solidified shell, via conduction through the solidified shell and is subsequently removed from the ingot surface via a number of mechanisms depending on position. Within the mould region, heat is transferred via contact conduction at the
meniscus and by conduction/convection through the gap that forms below the meniscus. Below the mould, the majority of sensible heat is extracted from the ingot by the impinging water stream. The magnitude of the heat flux at the point of water contact is such that the heat is conducted through the solid shell in both the axial and transverse directions and, hence, is referred to as being two-dimensional in nature. This phenomenon leads to the so-called 'advance cooling effect', where the shape of the isotherms within the ingot, while located in the mould, are affected predominately by heat transfer processes occurring at the point of water contact. As the magnitude of the heat flux levels off (further down the casting) the isotherms begin to parallel the ingot surface and heat flow approaches one-dimensional behaviour.

During startup, the heat flow pattern is more complex than at steady state. These differences are associated with the cast start procedure and the evolution of the temperature distribution as it approaches the steady state condition. The initial position of the starting block and platen prior to the cast start are shown in Figure 1.2. Casting commences by the introduction of molten metal into the system until the starting block is filled and the metal level reaches a specific height along the mould face. At this point, the platen is started downward at a controlled rate. This rate is gradually increased from the initial value to a nominal value, where it is held until the end of the cast. The water flow rate is also ramped up over the same period. These changes in both casting speed and flow rate are imposed as a means of controlling rate of heat extraction and hence the position of the solidus isotherm.
Ideally, the advanced cooling effect should extend up near the meniscus. This would reduce the deleterious effects on microstructure associated with transient mould cooling. Unfortunately, to achieve this extent of advanced cooling, production (low casting speed) and safety (potential for metal run out to over cooling the meniscus) are compromised. To achieve the balance required, the cast start procedure has been fine tuned largely by trial and error experimentation based on historical experience. Unfortunately, this qualitative approach to the cast startup, though enabling casting to be conducted with modest production rates and under relatively safe conditions, does not enhance our knowledge of the actual transient temperature evolution occurring during this period.

Figure 1.2. Initial position of platen and starting block.
The Trentwood plant of Kaiser Aluminum Corp., located in Spokane WA., produces rolled aluminum products for the beverage container industry. Included in the complex are D.C. casting facilities for producing ingots of AA5182 of nominal dimension 1680 mm x 800 mm in cross section. These ingots are used as feed stock in the subsequent rolling and fabrication operations for the production of beverage container lids. AA5182 is a non heat treatable aluminum alloy containing a nominal composition of magnesium 4.5 wt% with a small percentage of manganese (0.35 wt%) added to improve strength\(^1\). The binary phase diagram for the Al-Mg system\(^2\) (Figure 1.3) indicates that at this composition (solid line), magnesium remains in solid solution for the majority of the casting temperature cycle. The two phase boundary is crossed only at relatively low temperatures where diffusion constraints would limit the extent of Mg\(_2\)Al\(_3\) formation\(^1\) during the ingot cooling period. Therefore, strengthening by the formation of second phase precipitates (i.e. Mg\(_2\)Al\(_3\)) is insignificant and is generally confined to high Mg concentrations alloys and/or specialized heat treatments\(^1\). As a result, AA5182 is a relatively ductile alloy where strengthening is achieved primarily by work hardening. The high work hardening rate of AA5182 is illustrated by comparing the tensile strength of a fully annealed sample, 276 MPa (elongation to failure of 25%), with a highly cold worked material exhibiting a tensile strength of 412 MPa (with a corresponding decrease in strain to failure to 4%)\(^3\). The mechanical behaviour of the alloy in the cast condition is not known.
Figure 1.3 Binary phase diagram for aluminum - magnesium system.

Though AA5182 is relatively ductile, and is not generally susceptible to excessive second phase precipitation that may embrittle the material, cracking was still observed to occur during cast startup with this material in the vicinity of the starting block lip, along the base of the butt and along the surface of the long face. The face crack was deemed the most serious, as once initiated, could extend through the entire length of casting, rendering the ingot unsuitable for further processing.

The typical location of a surface face crack is illustrated in Figure 1.4. These cracks were observed to initiate at or near the center of the ingot rolling face in the vicinity of a transition that occurs between a lapped surface structure and an “exudated” surface morphology (photos of the surface morphologies are also included in Figure 1.4).
The difference in surface characteristics can be attributed to both the magnitude and duration of mould cooling experienced. The lapped surface results as a consequence of a high rate of heat extraction incurred over a relatively prolonged period. The lapped surface phenomena was only prevalent during the initial stages of startup. Conversely, the exudated surface is characteristic of minimal mould cooling associated with the formation of a gap between the metal and the mould extending for the majority of the mould length. The exudated surface morphology continues for the remainder of the casting. The surface transition was observed in all castings, regardless of whether cracking has occurred or not. Thus, it was unknown if the transition directly initiates cracking or whether the change in mould cooling or surface morphology influences heat flow patterns such that the propensity of cracking was increased.

Cracking of the form described above can be attenuated by a number of external parameters (metal cleanliness etc.), however, it is the generation of tensile thermal stresses which ultimately accounts for the initiation and growth of the face crack. Within the context of D.C. casting, thermal stresses arise due to constraints imposed on thermal contraction. These constraints manifest themselves at the local level (difference in temperature between interior and surface), but extends to the global scale, where differential contraction along the length of the ingot, in response to the temperature distribution, occurs. The high heat removal rate of the direct chill water would exaggerate differential thermal contraction and hence the thermal stresses that arise.
Figure 1.4  Schematic showing typical location of surface face cracks and surface morphology near cast start.
An observable effect of the stress generation due to differential thermal contraction, is macro ingot deformation in the form of butt curl. The genesis of butt curl begins at the point of first water contact with the ingot where the ingot surface is immediately cooled in relation to the remainder of the ingot. From our understanding of thermal stress generation, this leads to the generation of hoop stresses. However, due to the negligible amount of solidified metal that has formed, the hoop stresses generated at the surface of the ingot are partially relieved by upward displacement of the small ends of the ingot (butt curl). Some inward motion of the rolling faces can also occur, however, the exact nature of this form of deformation is not known. As casting proceeds, the amount of solidified material increases and the ability of the ingot to deform and relieve the hoop stresses decreases until butt curl stops.

To minimize the generation of the startup cracks due to thermal stresses, requires an understanding of first, the temperature behaviour during this period and secondly; the generation of thermal stresses and their evolution in relation to the temperature distribution and ingot deformation. However, the complexity of the startup procedure in terms of interaction between heat extraction, casting parameters and surface morphology and their effect on temperature and ultimately stress generation precludes "rule of thumb" and intuitive analysis. Thus a fundamental understanding of the behaviour in this region of the cast is required.
1.2 Background

The frequency of rejected ingots due to face cracking at the Trentwood facility was documented over an one year period and ranged from 4% to 20% in any given month. The variation in the number of cracked ingots occurred in a random fashion though a small correlation appears to exist between cracking frequency and a decrease in cooling water temperature with the onset of winter months. As the startup procedure remained constant over the reference period, the wide fluctuations in face cracking frequency indicates that the system used for casting AA5182 was very sensitive to small changes in external processing variables that may be occurring throughout the year. On this basis, a study was initiated by Kaiser Aluminum to correlate these processing variables with crack frequency.

As mentioned above, cooling water temperature was observed to vary throughout the year, hence, an experimental campaign was conducted to analyze this parameter in terms of both cracking frequency and magnitude of butt curl occurring during startup. These tests were conducted on a full scale casting pit at the Kaiser research facility in Pleasanton, California. The crack rate was observed to decrease as cooling water temperature was increased from 7 °C to 16 °C. With water temperatures above 16 °C, face cracking was eliminated. For this same range of water temperature the overall magnitude of butt curl was observed to increase as water temperature also increased. However, the correlation between butt curl magnitude and water temperature was relatively poor.
The effect of molten metal cleanliness was also analyzed. By minimizing the amount of entrained oxide entering the meniscus region, face cracking was eliminated regardless of water temperature. Both these findings with regards to water temperature and metal cleanliness, though useful in indicating potential areas of improvement within the casting facility, illustrate that a variable by variable analysis approach to reducing cracking was difficult due to the potential for multiple factors influencing the cracking behaviour. Therefore, the long term solution would be to alter the casting procedure itself, such that stresses during startup are reduced and the system becomes less sensitive, in terms of cracking, to perturbations in external variables.

To successfully manipulate the casting system, such that the desired thermal behaviour can be achieved, requires a fundamental knowledge of the process. However, as described in the introduction, the complexity of the startup procedure and the interaction between all the variables precludes an experimental campaign aimed at analyzing this phase. Therefore, a comprehensive study of the startup requires the use of a mathematical model capable of simulating both thermal and stress behavior. The general methodology of analyzing thermal stresses in complex systems by employing either a finite element or finite difference model is well documented. However, essential to this approach is an understanding of the boundary conditions that exist in the system.

Within the context of the D.C. cast start, the extraction of heat by the contact of the direct chill water with the ingot is of fundamental importance. This boundary is generally specified in the form of a water boiling curve such that the magnitude of flux is
only a function of surface temperature. However, the shape of the surface heat flux/surface temperature relation can be influenced by a number of factors such as; surface morphology, water flow rate and water jet configuration, therefore, it is necessary to establish the form of this curve specifically for the Trentwood casting conditions. Typically, boiling curve determination and analysis is based on thermal measurements from in situ thermocouples. Unfortunately, the methodologies available for calculating a representative system boiling curve from internal temperatures during the transient cast start are not well established.

The difficulties encountered in understanding the genesis of face cracking during the cast start are such that problem must be approached in a sequential manner. The following steps are deemed necessary to conduct a proper investigation into this form of defect generation. Firstly, a knowledge of the thermal conditions prevalent during cast startup is paramount. Secondly, strains and stresses arising due to this thermal behaviour must also be evaluated. Finally an in-depth study of cracking mechanisms correlating experimental data to the thermal stress analysis would be required. In view of the complexities associated with second step this work has focused on transient temperature development during the cast start and it's relation to crack generation and only a rudimentary stress analysis has been completed. From this understanding of thermal behaviour, design and optimization of the process, to reduce stresses, was initiated.
2. Literature review

A review of the literature was undertaken to accomplish several goals. Firstly, in view of the importance of the curve relating surface heat flux to surface temperature for direct water impingement in the DC casting process (system boiling curve), a comprehensive analysis of this relation is needed. This summary includes a review of water cooling heat transfer mechanisms, processing parameters influencing these mechanisms, the inverse calculation procedure used for determining the system boiling curves from internal temperature measurements and an analysis of this relation determined specifically for D.C. castings. Secondly, a review of defect generation during the cast start was undertaken with specific regard to crack generation and butt curl. Finally, the use of mathematical models as a tool for analyzing both thermal behaviour and stress generation during D.C. casting was discussed.

2.1 Mechanisms of Heat Transfer

To understand the evolution of the temperature distribution during cast startup, a knowledge of the heat extraction mechanisms occurring in the direct chill water cooling regime and, to a lesser extent, mould cooling region are required. This section discusses the physical mechanisms by which heat is extracted by the water and how these mechanisms are related to surface temperature in forming the system boiling curve. Included will be a discussion of the influence of surface morphology and water flow rate,
on the shape of this curve. A short overview of the mechanisms of mould cooling will also be presented.

2.1.1 Water Cooling

A typical heat flux vs. surface temperature relation for water cooling is shown schematically in Figure 2.1. In order of decreasing surface temperature, the four mechanisms of heat transfer illustrated are: film boiling, transition boiling, nucleate boiling and convective cooling. For the D.C. casting system, surface temperatures at the point of water contact place the heat transfer conditions in transition/film boiling region. As the ingot is cooled by the direct chill water, the amount of heat extracted follows the transition portion of the cooling curve up to the maximum value, at point A. With a further reduction in surface temperature, the intensity of nucleate boiling decreases (with a corresponding decrease in flux) until the surface temperature drops below the boiling point of water at which point heat is extracted by forced convective cooling.

Within the literature, extensive research has been conducted, under a variety of experimental conditions, with the aim of determining factors influencing the magnitude and range of the cooling mechanisms described above. In addition to this wealth of knowledge, the review papers by Dhir\(^4\) and Auracher\(^5\) on nucleate and transition boiling have provided significant insight into the fundamental mechanisms of boiling heat transfer. However, the direct applicability of the research cited towards enhancing our knowledge of the cooling conditions specific to a D.C. casting process is questionable. Therefore, a review of the literature, emphasizing factors influencing boiling behaviour, will attempt to
focus on research conducted under test conditions analogous to the D.C. process. This would include conditions encompassing flood contact of the surface by the fluid, transient cooling and, where possible, conditions of flowing fluid. Even within this restricted scope, experimental setups can significantly effect heat extraction behaviour\textsuperscript{4}, therefore only generalities, as opposed to specifics, on factors influencing system boiling curves will be presented.

![Diagram of heat flux vs. surface temperature relation for water cooling.](image)

Figure 2.1  Schematic of heat flux vs. surface temperature relation for water cooling.

2.1.1.1 Film Boiling

In the film boiling regime, heat is removed by conduction/convection through a continuous vapour layer existing between the surface and the cooling fluid. However, the
attainment of pure film boiling under normal D.C. casting conditions is unlikely as sufficient cooling imparted by the impinging water precludes the development of a continuous vapour film at any point along the ingot. Therefore, for all practical purposes, the mechanism of heat extraction through a vapour film will be considered only as it pertains to the transition cooling regime.

2.1.1.2 Transition Boiling

Transition boiling exhibits the characteristics of both film and nucleate boiling. Mechanistically this entails an intermittent combination of vapour film formation and direct fluid/surface contact, with the proportion of the later increasing with decreasing surface temperature. For direct fluid contact, heat is extracted by intense boiling of the cooling fluid and is a more efficient mechanism of heat transfer than convection/conduction across a vapour barrier. Thus, the shape of this portion of the boiling curve is directly related to the amount of direct fluid /surface contact occurring. Intuitively, changes in the system that increase the propensity for water contact with the surface would also increase the magnitude of flux at any temperature. For bench scale experiments, increasing the mass flow rate or velocity of the cooling fluid passing over the surface, was observed to enhance the magnitude of heat extracted at all surface temperatures. The temperature at which the maximum flux value (point A in Figure 2.1) occurred in these experiments also increased.

In addition to fluid flow, the surface morphology can influence the shape of the transition portion of the cooling curve. In tests under pool boiling conditions, using
water\textsuperscript{4,10}, acetone\textsuperscript{5} and pentane\textsuperscript{9} cooling fluids, increasing surface roughness shifted the position of the maximum flux (point A) to lower temperatures. This behaviour could be attributed to the increased surface roughness enhancing vapour film stability at the surface. Though the surface temperature at which the peak flux occurred decreased with increasing roughness, the heat flux value either remained equal\textsuperscript{4}, increased\textsuperscript{9} or decreased\textsuperscript{5,10} in response to increasing surface roughness. The relationship between both mass flow rate and surface roughness and its effects on the cooling curve is not known.

The extent of water subcooling (difference between initial temperature of cooling water and its boiling temperature) can influence the shape of the transition flux curve. A study by Cheng et al.\textsuperscript{6} conducted under conditions of forced water flow, showed an increase in the magnitude of flux along the entire transition curve as the amount of subcooling increased from 0 to 27.8 °C. Similar behaviour was observed by Ma et al.\textsuperscript{11} on an experimental apparatus used to characterize the jet impingement of water on hot rolled steel and by Bamberger et al.\textsuperscript{12} and Dhir\textsuperscript{4} in water pool boiling studies. For all four studies, the temperature of the peak flux shifted to higher temperatures with increasing amounts of subcooling. Unfortunately, in the studies involving water flow, the maximum value of subcooling examined was 27.8 °C (26.8 °C for Ma et al.\textsuperscript{11} and 27.8 °C for Cheng et al.\textsuperscript{6}) which is considerably less than the 80 °C subcooling typical in D.C. casting.

\subsection*{2.1.1.3 Nucleate Boiling}

At the peak heat flux (point A Figure 2.1) value, the mechanism of heat extraction shifts from transition to nucleate boiling. This change in heat transfer mechanism is
characterized by the continuous contact of cooling fluid with the surface. Heat is removed from the body by the generation and subsequent detachment and condensation of vapour bubbles from the surface to the bulk volume of fluid. As the surface temperature decreases, the rate of bubble nucleation and detachment also decreases with a resulting drop in heat extraction.

For transient cooling conditions, the magnitude of the peak flux $A$ does not necessarily represent the maximum flux possible by a nucleate boiling mechanism, but only the intensity of bubble generation and detachment present when transition boiling ends. Thus, the start of nucleate boiling (magnitude and temperature of Point $A$) is dependent on conditions which influence the cessation of transition boiling. These conditions, specifically mass flow rate/velocity and surface condition have been discussed above. Within the nucleate boiling regime itself, the slope of the boiling curve is not significantly influenced by fluid flow$^6,7,9$ and/or by water subcooling.$^4$ However, as the surface temperatures approaches the boiling point of cooling fluid (with a corresponding decrease in the intensity of nucleate boiling), the influence of convective cooling increases. Thus factors affecting convective cooling (such as fluid flow and fluid subcooling) begin to influence$^4,9$ the magnitude of nucleate boiling curve in this regime.

Conversely, surface morphology can have a significant effect on the slope of the nucleate boiling curve. In several experiments conducted under pool boiling conditions, increasing surface roughness was observed to increase the slope of the nucleate boiling curve substantially$^9,10$. These tests indicated that the increased roughness enhanced vapour
bubble nucleation, thereby increasing the heat removal rate at surface temperatures near
the boiling point.

2.1.1.4 Convective Cooling

At surface temperatures below the boiling point of the fluid, heat is extracted entirely by forced convection. Equations describing this type of heat transfer have been well developed.\textsuperscript{9,13} Water flow rate, through its effect on the Reynolds number of the moving fluid\textsuperscript{13}, is considered a dominate factor. By increasing fluid flow, the heat extracted by the water at a particular surface temperature is observed to increase.\textsuperscript{9,13} Also, the rate of heat transfer is proportional to the amount of fluid subcooling.\textsuperscript{4} Through the effects described above, convective cooling behaviour influences both the magnitude of flux at the transition point (Point B in Figure 2.1) between nucleate boiling and forced convection cooling and the slope of the flux curve below the fluid boiling point.

2.1.2 Mould Cooling

Fundamental work on the mechanisms of mould cooling has been analyzed in relation to foundry casting procedures.\textsuperscript{25,26} The heat transfer coefficients calculated for a metal solidifying against a metallic mould are observed to vary as a function of time. The temporal variation is directly related to the amount of direct metal / mould interaction. A high heat transfer coefficient is observed for conditions of intimate metal/mould contact. As the metal solidifies it begins to contract away from the mould resulting in the formation of an air gap resulting in a substantial decrease in heat transfer. The peak heat transfer
coefficient observed for aluminum contacting a chilled mould\textsuperscript{25,26} ranges from 2000-4000 W/m\textsuperscript{2} K. This value levels off at approximately 200-500 W/m\textsuperscript{2} K following air gap formation. Under these conditions, heat is transferred primarily through conduction / convection across the gap.

2.2 Inverse Heat Calculations

The heat flux/surface temperature data generated from the experiments described above are useful in indicating trends in how various variables influence boiling curve shape. However, it is virtually impossible to reproduce actual casting conditions in laboratory scale experiments. Consequently, heat flux/surface temperature relations are typically calculated from internal temperature measurements of the actual system being studied. The procedure to determine heat transfer conditions based on internal temperatures is known as the Inverse Heat Calculation (IHC) method\textsuperscript{27}. The IHC procedure can be applied to a variety of problems, however, in view of the thermal behaviour prevalent at the cast start, only solutions for transient conditions are applicable. Towards our understanding of the general inverse technique, this section outlines the general formulation of the IHC methodology followed by a review of the techniques applied in determining the cooling curve in a D.C. cast system.

2.2.1 General Formulation of Inverse Heat Calculations

The transient IHC problem, is considered ill-posed or ill-conditioned, as a multiple number of surface fluxes could account for the variation in interior temperatures observed.
This “multiplicity” makes the problem very difficult to solve by a direct mathematical solution\textsuperscript{16}. As such, the IHC calculations generally require a method by which the unknown thermal conditions can be predicted. This predictive capability is achieved by employing a numerical technique such as the finite element or finite difference method\textsuperscript{28,29}.

The basic concept of the numerical IHC solutions is the application of boundary conditions such that the difference between the measured internal temperatures and the numerical solution, at the same location are minimized. Sophisticated techniques have been developed for the one-dimensional transient problem, that impose a surface flux based on the temperature evolution over several “future” time steps\textsuperscript{28}. This procedure helps to minimize the effect of thermal delay between the boundary and the response of the interior temperature. However, the complexity of the relations between interior temperature and imposed surface flux increases significantly for a transient two-dimensional problem where thermal response at any one location is dependent on its relative position. To solve this form of problem, several approaches have been proposed in the literature.

For the specific circumstance of a fixed heat flux distribution imposed on a two-dimensional body, it is possible to subdivide the surface into a number of discretized segments\textsuperscript{30} over which the flux was assumed to be constant. Typically the number of segments would correspond to the number of internal temperature measurements. The applied fluxes, in each discretized region, were simultaneously altered based on the difference between the numerical and measured temperatures and a location dependent
sensitivity coefficient. Alternatively, Reinhardt\textsuperscript{31} extended Beck's\textsuperscript{28} one dimensional IHC analysis by approximating the two dimensional problem as a series of decoupled one dimensional problems. It was indicated that the method was applicable to data obtained only from specially designed and instrumented bodies.

2.2.2 Inverse Heat Calculations in D.C. Casting

A direct application of the two dimensional IHC methods described above, has not, based on a review of the literature, been applied to the D.C. casting system. However, several methods including a subset of the general IHC methodology have been used in the examination of heat transfer in the D.C. casting system. This section will include firstly, a description of the methodologies employed for calculating the heat flux/surface temperature in actual casting systems. Secondly, the calculated system boiling curves themselves will be compared and where possible the effects of casting parameters on their shape discussed.

In a relevant study, Weckman \textit{et al.}\textsuperscript{13} utilized what may be described as a subset of the inverse heat conduction (IHC) methodology in analyzing the heat flows in a 155 mm D.C. cast billet of AA6063. Their technique employed a two-dimensional, finite element based, steady state heat conduction model with Dirichlet type boundary conditions applied to the top and bottom of the billet. In addition, the position of the solid/liquidus interface, and the associated latent heat of fusion, was assumed beforehand and fixed positionally in the simulation. For the boundary representing the water cooled face of the billet, fixed surface temperatures were employed in the model. These surface temperatures were then
adjusted by a trial-and-error process until the difference between the measured and calculated thermal responses were minimized. Based on the calculated surface temperatures, flux values were then determined and the boiling curve of the system was established. A drawback of this approach, was that the temperature distribution within the billet was artificially constrained by the position of the solidification interface. Further, the analysis was limited to an investigation of the steady state heat conditions.

In a different study on a 155mm diameter billet of AA6063, Grandfield et al.\textsuperscript{32} directly calculated the amount of heat extracted axially along the billet surface by measuring the temperature profile of the direct chill water. Unfortunately, the methodology used in obtaining the water temperature profile and the subsequent heat flux profile was not described. Once obtained, the calculated flux was then correlated with the measured surface temperature profile to obtain a system cooling curve.

An alternative procedure was developed by Bakken et al.\textsuperscript{33} for calculating the heat flux/surface temperature relation in the direct chill water regime. Their method was based on an analytical solution to a steady state heat balance for a small fixed volume of material at a surface location. The calculation is based on an estimation of the surface temperature from 3 interior thermocouples using a collocation interpolation technique. To minimize the interpolation error, a special jig was developed to ensure that the thermocouples were placed near the surface and axially aligned with each other. From the estimated surface temperature, and the solution to the steady state heat flux equation, a characteristic cooling curve could be calculated.
2.2.2.1 Analysis of Calculated Heat Flux/Surface Temperature Relations

The heat flux/surface temperature relations determined for several D.C. cast systems, are presented in Figure 2.2. The differences between the curves may indicate in part that the flux surface temperature relations are a strong function of the specific casting system being analyzed and/or alternatively, the solution is dependent on the IHC methodology. To help understand the differences in each system, parameters influencing the form of the individual curves are discussed. Weckman et al.\textsuperscript{13} indicated that the magnitude of flux, in the convective regime and during the early stages of nucleate boiling, was proportional to water flow rate. Baken et al.\textsuperscript{33} discussed the effect of surface temperature and casting speed on the magnitude of the peak flux. Both the temperature and magnitude of the maximum flux was found to depend on cooling water flow rate, the water jet geometry and water subcooling, though specific details of the contribution of each were not discussed. The authors\textsuperscript{33} also indicated that maximum flux increased as the casting speed was increased. It was suggested that with a higher casting speed, the amount of sensible heat available increased, hence, the maximum flux also increases. The mechanisms by which additional heat, at a given surface temperature was extracted were not elaborated on. Jensen et al.\textsuperscript{34} employed the inverse calculation technique developed by Bakken et al.\textsuperscript{33} to determine the cooling curves for several sizes of AA6063 extrusion billets. A variation in water flow from 83 to 93 l/min did not appreciably influence the shape of the system boiling curves calculated for a 178 mm diameter billet.
Grandfield et al.\textsuperscript{132} discussed the effects of water temperature, water impingement intensity and water flow rate on the measured surface temperature of a 155 mm diameter 6063 casting. Qualitatively, it was observed that water temperature, ranging from 20-35 °C, had negligible effect on surface temperature in the water boiling regime, although the final billet surface temperature was observed to decrease slightly for the lower water temperature. Increasing the water flow rate from 60 to 120 l/min was observed to decrease surface temperature, at comparable locations below the water impact point, but only in the region where the surface temperature approached 100 °C. The most significant effect on surface temperature was observed when cooling intensity was reduced by incorporation of CO\textsubscript{2} gas into the cooling water or by using a mist spray as opposed to a water jet. The reduction in flux intensity resulted in a considerable delay following water contact before the surface temperature cooled below 400 °C. The overall effects of these parametric changes on the heat flux/surface temperature relation were not presented.
2.3 Defect Generation

The majority of analyzes regarding defects observed during startup of rolling ingots has concentrated on butt curl. Though butt curl itself can be considered a macro defect, its manifestation in large rolling ingots can lead to a number of other defects\textsuperscript{35,36} or difficulties in the casting process. These can range from butt swell, cold shutting, segregation, ingot deformity and to safety considerations such as run out of melt or ingot hang-up. Research has focused primarily on controlling the magnitude of butt curl, however, as this phenomena is directly related to stress generation and ultimately thermal behaviour during startup a review of this defect was deemed necessary. Though the mechanisms of surface face cracking have not been specifically discussed within the
literature, a general review of the forms of crack generation during D.C. casting will also be presented.

2.3.1 Butt Curl

The genesis of butt curl has already been discussed in the introduction, thus the review will focus on techniques employed to control this phenomena. These range from adjustment of the process parameters, such as casting speed and water flow, to physically altering the cooling intensity by addition of CO$_2$ gas or by employing pulsed water. An investigation by Droste et al.$^{35}$ analyzed the effect of casting velocity, water flow and alloy type on butt curl. It was observed that the overall magnitude of butt curl was proportional to casting velocity, but cooling water volume was of minor importance except at extreme casting conditions (i.e. high cast velocity and low water flow). However, details at these extreme conditions were not given.

Alternatively, casting procedures that directly alter the intensity of water cooling have been utilized to control butt curl. In one such technique$^{36}$, CO$_2$ gas was dissolved in the direct chill cooling water. The dissolved CO$_2$ evolves as gas bubbles as the water exits the mould. In a manner analogous to the vapour film in the transition boiling regime, these bubbles can then act as an insulating barrier and reduce the intensity of water cooling. As a consequence, the amount of butt curl was reduced.

In a manner analogous to the CO$_2$ gas method, Bryson$^{37}$ modified the water delivery system such that the water jet could be turned on and off or "pulsed" onto the
surface. By manipulating the pulse sequence, the overall contact time of water with the ingot was reduced with an accompanying decrease in the amount of heat extracted. This technique was also observed to reduced butt curl. These studies would indicate that a reduction in heat flow is necessary to reduce butt curl, however, the effect of these conditions on stress generation are not known.

2.3.2 Cracking Mechanisms

The modes of cracking in D.C. cast ingots or billets are considered to take one of two forms; hot cracking (tearing) or cold cracking. Hot tearing occurs at temperatures in the solidification range of the alloy and is characterized by intragranular cracking. The high temperature cracks can initiate at regions of solute segregation or in regions where solidification shrinkage cannot be eliminated by metal afterflow. Conversely, cold cracks occurs at much lower temperatures and are typically associated with high residual stresses. Excessive residual stresses generally occur in high strength alloys where material deformation would be insufficient to relieve the effects of differential thermal contraction. The cold cracks are believed to initiate at micro defects such as inclusions or microcavities.

2.4 Mathematical Models

Mathematical simulations have been used extensively to analyze temperature distribution and stress generation in D.C. castings. The number of references precludes
an exhaustive analysis of all material, thus, the focus of this review will be confined to the simulation analysis encompassing the startup phase\textsuperscript{40,49-54}.

Hannart et al.\textsuperscript{40} studied the evolution of thermal stress during startup of a 1500 x 500 mm AA2024 ingot. Thermal boundary conditions included heat transfer coefficients for both mould and direct chill cooling and a heat flux between the starting block and the bottom of the ingot. Values for these boundary conditions were not given. Temperature evolution during startup was presented as contour profiles for the entire ingot. As a result, localized thermal behaviour at the ingot face could not be analyzed. Included in the simulation study was a full three dimensional stress analysis. The solid aluminum in the stress portion of the analysis was treated as an elastic-plastic strain rate dependent isotropic material. This mechanical behaviour was described by an empirical constitutive equation determined from tensile testing. The authors\textsuperscript{40} observed a peak tensile stress in the neighborhood of the small faces of the ingot. This was indicated as a likely location for crack propagation. Calculated butt curl, from the simulation, was compared to a measured value as a means of qualitatively assessing the correctness of the stress model.

Krahenbuhl et al.\textsuperscript{49} employed a numerical model to optimize mould position during the startup phase of an EMC (Electro Magnetic Casting) cast ingot of 5182 with dimensions of 380 x 2080 mm. The numerical simulation included the effects of the electromagnetic field and fluid flow. Negligible information was presented regarding the boundary conditions employed in the thermal portion of the model and the resulting temperature distribution.
Mariaux et al. developed a mathematical model to study the transient thermomechanical behaviour of a 380 x 2080 mm EMC cast ingot. Thermal boundaries included Neumann conditions for both the direct chill water and the mould or starting block regions of the ingot. Values for the water heat transfer coefficient were not given. Temperature data from the startup was presented as contour maps encompassing the entire ingot, therefore localized thermal behaviour at specific locations could not be analyzed. Viscoplastic deformation in the stress analysis was described using a creep relationship, where strain rate behaviour was calculated as a function of both temperature and stress. Unfortunately the stress modelling was performed using only a two dimensional system, which has limited applicability to a three-dimensional ingot.

Jensen et al. employed a two-dimensional thermal model to analyze the mechanisms of hot centreline cracking in AA6063 (204 mm diameter) billets. Calculated sump depth was used as an indicator of crack propensity in which a deep sump was associated with a high propensity for cracking. The shape of the boiling curve used to represent the direct water cooling was not included in the paper.

Fjaer et al. employed a three dimensional thermal stress model to examine the effect of starting block design on butt curl deformation in a rolling sheet ingot. In this study, calculated butt curl was observed to be sensitive to the thermal boundary conditions applied in the FEM model. Unfortunately, specific details of the boundary conditions employed were not given. The stress data shown was limited to the initial stages of casting with the largest stresses found in the region of water impingement. The development of
stresses further along the casting that may lead to face cracking were not elaborated on. In addition, specifics regarding the intricacies of three-dimensional stress modelling were also not discussed.

Drezet et al.\textsuperscript{54} employed the commercial FEM model ABAQUS to establish the effect of casting parameters on deformation during startup. Modelling was conducted on a two-dimensional axial slice at the centerline of a rolling sheet ingot. Specifics with regards to stress development that may lead to face cracking were not elaborated on. Also the direct chill water boundary condition employed in the analysis was also not discussed.

A review of the literature indicates that the problem of surface face cracking (of the form described in the introduction) during startup of an AA5182 ingot has not been specifically addressed. However, mathematical simulations of the startup procedure in terms of both thermal behaviour and stress generation indicate the usefulness of this technique for understanding ingot behaviour in this portion of the casting. Essential to the usefulness of these models are the inclusion of suitable heat flux boundary conditions. Unfortunately, a detailed description of the system boiling curves employed in the simulation studies was not included. Whether the exclusion of this information stems from the proprietary nature of the system boiling curves or from a general lack of knowledge is not known. In summation, the basic tools or methods required to analyze the problem of face cracking are available, however, specifics, such as the form of the heat flux/surface temperature relation for water cooling are lacking.
3. Scope and Objectives

3.1 Scope of the Research Programme

The purpose of this investigation was to enhance our understanding of the thermal conditions existing during the startup phase when D.C. casting a rolling ingot of AA5182 aluminum. The resulting knowledge has been analyzed with the aim of reducing the propensity for face cracking during this period. However, due to the complexity of the cast start, it was necessary to examine thermal behaviour and stress generation by way of a mathematical model. Mathematical models have been used by other researchers to analyze cracking in equally complex systems such as refractory brick production or the static casting of steel ingots. Essential to all numerical simulations, are the inclusion of thermal boundary conditions that are representative of the process being considered. Unfortunately, direct measurement of heat transfer conditions, especially in the direct chill water zone in D.C. casting, are difficult. Therefore, an indirect technique, based on internal temperature measurements was adopted.

As part of the study, an experimental campaign was initiated in which thermocouples were embedded into a full size rolling ingot of AA5182 during the cast start. In addition to temperature, water flow rates and platform position were monitored. Also included in the measurements was the amount of ingot deformation or butt curl that was occurring.
In order to interpret the results of the experimental study a methodology was developed by which the temperature dependence of heat transfer to the direct chill water prevalent during the cast start could be determined from the internal temperature measurements. This procedure employs a finite element heat conduction model for predicting the heat flow conditions. Once calculated the representative heat flux relations enhance our understanding of the interaction between the direct chill water and the solidifying ingot. This knowledge is essential when making subsequent modification or design changes to the casting process.

The finite element method was chosen for the analysis methodology primarily as the mathematical solving routines were already developed "in house" thus enabling access to the finite element code. A second advantage of the finite element method is the relative ease of incorporating thermal data directly into a stress analysis. Access to the FEM routines proved essential as modification to the peripheral components of the primary solver were necessary in calculating the heat flow conditions in the direct chill water regime. In this respect, the flexibility of an “in house” finite element program greatly outweighed the benefits of commercial simulation packages available at the commencement of this research.

In addition to being applied in the surface heat flux calculation methodology, the finite element routines were modified to simulate the thermal conditions at the cast start procedure in both two and three dimensions. The two-dimensional calculations were employed to validate the veracity of the model by comparing the simulation thermal
behaviour with the measured temperatures. The three-dimensional thermal model was then used as input into a three-dimensional stress simulation. The three-dimensional model proved necessary to properly account for the global effects of differential thermal contraction.

Based on the results of the finite element simulations an intensive analysis of thermal behaviour was undertaken to determine conditions conducive to cracking. Changes in the process that would minimize the potential for cracking were then recommended.

3.2 Objectives of the Research Programme

The objectives of the research programme can be summarized as follows:

[1] To develop a methodology capable of determining the heat transfer conditions in the direct water contact regime. The procedure must be sufficiently general such that it can be applied to the cast start and only require as input the temperature behaviour from a single thermocouple.

[2] To formulate, develop and validate a mathematical model capable of simulating the thermal behaviour in a D.C. cast ingot during startup.

[3] To analyze both thermal behaviour and stress generation with the aim of determining conditions conducive to face cracking.
Based on our knowledge of [1 -3], propose changes to the casting system and process parameters that would attenuate the sensitivity of the casting process to crack formation.
4. Industrial Measurements

To achieve the objectives outlined in the previous chapter, it was necessary to obtain experimental data from an industrial size D.C. casting of AA5182 aluminum. Two sets of industrial trials were conducted at the Kaiser Aluminum Research facility in Pleasanton, California. The purpose of the trials was to obtain relevant temperature measurements and casting data for determining the heat flow conditions during the cast startup and for validating both a two and three dimensional heat transfer and stress model used in the analysis.

4.1 Experimental Technique

The experimental technique was relatively straightforward and involved placement of thermocouples into a 1680 x 800 mm ingot during startup. For the purpose of presenting the data, the two industrial trials will be considered separately. Unfortunately, due to experimental difficulties, only portions of the data from the first casting campaign could be incorporated into the broader study of ingot thermal behaviour. The temperature data gathered from thermocouples placed in the base of the ingot during this first round of casts were utilized only in empirical calculations describing the relation between bottom ingot cooling and butt curl. These calculations will be discussed in a subsequent chapter. The location of the base thermocouples are presented in Figure A.1 in Appendix A. The temperature data obtained from the three castings conducted in this initial campaign are presented in Figures A.2 - A.4. Included in the temperature data graphs are the base
deflection or butt curl values measured at one end of the ingot. The experimental technique used to obtain these values was relatively unsophisticated, however, the butt measurement technique was improved considerably in the second set of casting trials.

Of more importance are the thermal measurement obtained from the second casting trial. These experiments entailed positioning of thermocouples along the broad face of the ingot for two of three casts and into the ingot base for a final cast. The broad face thermocouples were organized into groups consisting of three pairs of thermocouples positioned in the ingot such that following criteria were met:

[1] heat flow, along a plane parallel to the axial direction and perpendicular to the surface, was two dimensional.

[2] the full spectrum of conditions experienced during startup were encompassed

To ensure a two-dimensional heat flow, the two thermocouple groups inserted in each face cast were positioned at the locations illustrated in Figure 4.1. These thermocouple locations avoid the three-dimensional heat flow experienced at the ingot corners. The center thermocouple group ensured that the thermal conditions in the vicinity of crack were analyzed. The location of the second thermocouple group was primarily to provide verification of the consistency of heat flow along the broad face of the ingot.
As mentioned in the introduction, standard starting practice entails both a variation in casting speed and in water flow rate. In addition, the surface morphology was also observed to change (see Figure 1.4). Therefore, the thermocouples pairs in each group were placed such that the entire range of casting conditions were covered. Figure 4.2 illustrates the approximate axial location of the thermocouple pairs in each group. The casting conditions experienced at all three locations (B, M and T) are presented in Table 4.1. Of particular note, the B thermocouple pair experiences low water flow and a lapped
surface while at the location of the T pair, the water flow is high and the surface morphology is exudated. The thermocouples at each axial locations are defined as TC1 (closest to surface) and TC2 (more distant from surface). Though (as will be discussed in Chapter 6) TC1 was only required in the heat flux analysis, TC2 was included to provide both an independent verification of the heat flux calculations and for verification of the models subsequently employed.

Figure 4.2 Longitudinal view schematic showing axial location of thermocouple pairs in each face group.
Table 4.1

Casting conditions experienced at face thermocouple pairs

<table>
<thead>
<tr>
<th>TC Position</th>
<th>Cast Velocity (mm/s)</th>
<th>Water Flow (l/sm)</th>
<th>Surface Morphology</th>
</tr>
</thead>
<tbody>
<tr>
<td>B</td>
<td>0.77 - 0.899</td>
<td>1.97 - 3.33</td>
<td>lapped</td>
</tr>
<tr>
<td>M</td>
<td>0.899</td>
<td>1.97 - 3.33</td>
<td>transition</td>
</tr>
<tr>
<td>T</td>
<td>0.899</td>
<td>3.33</td>
<td>exudated</td>
</tr>
</tbody>
</table>

Following the standard practice of Kaiser Research, Type - K, Nickel - Chromium vs. Nickel-Aluminum thermocouples of size 0.02 in. (0.5mm) were selected for placement into the ingot. As seen in Figure 4.2, the six thermocouples in each group were attached to a leader wire and inserted such that the exposed thermocouple junction was parallel to the ingot surface. To ensure adequate contact with the molten aluminum, the junction was braided for a length of 3 mm and mechanically crimped at the end. The thermocouple leads were then connected to a central data acquisition system and thermocouple voltage was recorded at the maximum data logging rate once every 3 seconds. Included in the measured data, was the casting time and platen position. In addition, dynamic displacement measurements were obtained from two motion transducers located at the center of each of the small ends of the ingot. These transducers measured the movement of a reference rod that was solidified into the ingot. Based on this measured motion and the recorded platen position, a measure of dynamic butt curl was obtained.
In addition to analyzing the heat flow conditions in the direct chill water region, a cast was conducted with thermocouples placed along the bottom of the ingot. The purpose of this cast was firstly; to determine the thermal behaviour in the ingot bottom during contact cooling with the starting block and secondly; to qualitatively assess the extent of cooling arising due to penetration of water between the ingot and the starting block. Typically, the direct chill water applied to the ingot faces will flow down the ingot and remain on the outside of the starting block, however, ingot deformation in the form of butt curl is of sufficient magnitude to modify water flow patterns such that some water flowing down the short end face is directed underneath the ingot where it enhances cooling. Modelling of the cast start must include some measure of this additional cooling. The location of the thermocouples placed in the base of the casting are shown in Figure 4.3.

![Figure 4.3 Transverse view schematic of ingot quarter showing location of base thermocouples.](image)
4.2 Experimental Procedure

In total three casts were instrumented. A single cast was used to monitor the ingot base thermal behaviour with the two remaining casts devoted to the face thermocouple groups. All three casts were repeated under identical starting conditions and also similar locations with regard to the placement of the face thermocouples groups. The only difference between the castings was the temperature of the cooling water. Cast 1, of the face thermocouple group, was subjected to a water temperature of 8.9 °C in comparison to a temperature of 19.4 °C for both the second face and the base thermocouple casts. Metal temperature in the inlet trough was maintained at approximately 690 °C. Water hardness remained at a constant value of 65 PPM. Following casting, the sections of ingot containing the thermocouples were extracted and machined to determine the location of the thermocouple beads.

4.3 Data Analysis

The casting data recorded was analyzed back at UBC. It became quickly apparent that some of the thermocouple data collected was faulty. The questionable temperature data was attributed primarily to unsatisfactory entrainment of the thermocouple lead into the metal (where observed in the post casting autopsy) and due to electronic malfunctions in the cases of both Cast1 - Center M - TC1 (see Figure 4.5) and Cast2 - Offset M -TC1. The fluctuations observed in the responses of both these thermocouples was believed to be nonsensical as the thermal behaviour observed was not mirrored in the accompanying TC2...
temperatures. In total, the temperature responses of five thermocouples were rejected and were not considered in any subsequent analysis.

Representative examples of the measured face thermocouple data are presented in Figures 4.4, 4.5 and 4.6. These curves are for the center thermocouple group from Cast 1 and represent the B, M and T pairs respectively. The ordinate axis represents time since the start of casting or more correctly, the beginning of platen motion. Also included in the graphs are lines representing the casting times at which the axial location of the thermocouple pairs exit the mould and enters the direct chill water zone. Some salient features of the data are the rapid drops in temperature observed as the thermocouples enters the direct chill water zone. In addition, the thermocouples B-TC1 and M-TC1 also experienced an observable degree of mould cooling. The temperature cusp observed with these thermocouples is attributed to a high rate of mould cooling (rapid drop in temperature) followed by a subsequent rebound as contact with the mould (with a corresponding decrease in the rate of heat extraction) was lost. The lapped surface morphology exhibited at the B and M pair locations confirms the occurrence of a high degree of mould/metal interaction. The lack of any thermal cusps in the T zone data (Figure 4.6) indicate the exudated surface morphology observed in this region is characteristic of minimal mould/metal contact.

The sudden decrease in temperature observed for M-TC1 at 400 °C was believed to result from an electronic malfunction as an actual thermal response at this location would be mirrored to a certain extent by M-TC2. Overall the general characteristics
exhibited by these temperature curves are consistent with the remaining 3 face thermocouple groups. The temperature data for these groups are graphed in Figures A.5 to A.7 in Appendix A.

![Temperature Response Graph](image)

Figure 4.4 Temperature response observed for thermocouples TC1 and TC2 located at the face center and B location for Cast 1 (Cast 1 - Centre B).
Figure 4.5  Temperature response observed for thermocouples TC1 and TC2 located at the face center and M location for Cast 1 (Cast 1 - Centre M).

Figure 4.6  Temperature response observed for thermocouples TC1 and TC2 located at the face center and T location for Cast 1 (Cast 1 - Centre T).
An example of temperature behaviour recorded in the ingot base is illustrated in Figure 4.7. These curves represent data from thermocouples located at positions 3 and 4 in Figure 4.3. The zero casting time represents the initial conveyance of metal into the starting block. Within the graph the observed thermocouple responses shown can be divided into 3 distinct regimes. From $t = 0$ to 145 temperature is observed to decrease gradually indicating a low to moderate rate of heat extraction. At approximately 145 seconds, the temperatures are observed to rebound slightly. This behaviour would indicates a further drop in the heat transfer between the ingot base and the starting block. The beginning of butt curl (as the water contacts the ingot faces) and the subsequent lifting of the ingot away from the starting block may account for this phenomena. At approximately 225 seconds a rapid drop in temperature occurs. This is associated with the penetration of direct chill water beneath the ingot enhancing the heat transfer. The rebound in temperature at 240 seconds indicates a temporary loss of contact with the water followed by another rapid drop in temperature as water contact is reestablished (the exact mechanism to account for this rebound is not known). Similar temperature profiles are observed for all the base thermocouples (these curves are presented in Figure A.8 - A.9 in Appendix A), however the temporal occurrence and magnitude of each of the events described above varies according to thermocouple location with respect to the short end of the ingot. Base thermocouple results from the first casting campaign (see Appendix A) exhibited similar behaviour. However, results from these tests indicate water cooling does not extend to all locations along the ingot bottom. Portions of the ingot
bottom in the vicinity of the geometric center of the ingot are observed to cool at a much lower rate indicating negligible water contact.

![Temperature vs Time Graph](image)

**Figure 4.7** Measured temperature at bottom thermocouple locations 3 and 4.

The butt curl measured during the base thermocouple cast is shown in Figure 4.8. The two lines represent the values measured at the short ends of the ingot which are defined as North and South. Time zero time corresponds to the molten metal initially entering the starting block. Butt curl begins at approximately 150 sec, which correlates well with the time at which the starting block first leaves the mould. At 180 seconds the butt curl rate escalates and remains at a relatively constant value until it begins to levels off at 320 sec. The rapid increase in butt curl rate is believed to be associated with the establishment of a critical length of ingot exposed to the direct chill cooling water. The
leveling off is attributed to the constraint imposed on macro deformation by the increasing amount of solidified metal that has formed by this stage in the casting. The differences in final ingot deformation at either end are attributed to experimental error.

The butt curl observed at the narrow end of the ingot for the face thermocouple casts are compared in Figure 4.9. The only difference between the two casts was the temperature of the direct chill water. Zero time in this graph corresponds to the start of platen drop with the starting block first leaving the ingot at 24 seconds. The butt curl measured from the south end of the ingot for each cast is indicated. In general the measured curves exhibit similar behaviour in terms of rate of change of butt curl versus time in both the initial region and during the leveling off period. However, a significant difference is observed between the curves of each cast with regards to the overall magnitude of butt curl. Unfortunately, the large variation in measured butt curl (between North and South) for the first face cast (water $T = 8.8 \, ^{\circ}\text{C}$) coupled with a lack of supporting data precludes assessing the influence of water temperature on the overall magnitude of butt curl.

4.3.1 Ingot Autopsy

Following casting, the portions of the ingot containing the thermocouple groups were removed and machined to determine the location of each thermocouple tip. The face thermocouple positions were defined both by the distance of the thermocouple from the surface and it’s axial location above the bottom of the casting face (commonly referred to as the ingot lip). The results of the autopsy are tabulated in Table A.1 in Appendix A.
Similarly the bottom thermocouples are defined by the distance above ingot bottom and from the center of the casting. The locations of these thermocouples are summarized in Table A.2 in Appendix A. Both tables also indicate those thermocouples that experienced electronic malfunction or were observed not to be entrained in the ingot.

![Figure 4.8](image_url) Measured butt curl at narrow ends of ingot as a function of total casting time for the base thermocouple instrumentation cast.
4.3.2 Surface Morphology

The surface morphology observed for all the face thermocouple groups is consistent with the photograph presented in Figure 1.4. This includes a lapped surface at the start followed by an exuded surface that extends for the remainder of the casting. However, subtle differences do exist in both the micro morphology of the lapped surface and the distance of the transition from the casting bottom lip. The lapped structure at the ingot center exhibits well defined and relatively smooth metal/mould contacts spaced at 10-20mm. The morphology at the offset thermocouple group shows less defined laps with a slightly less smooth surface. The differences are attributed to the severity of contact cooling with the mould. A microphotograph of the offset lapped region is presented in Figure 4.10. The rule numbers indicate distance above the face lip in mm.
The range of the lapped region (distance from ingot lip to beginning of transition) was observed to differ between the center and offset ingot locations. At the center of the ingot the lapped surface extends for 160 mm for face Cast 1 and 168 mm for face Cast 2. Conversely, at offset thermocouple groups the lapped structure was measured at 130 mm for face Cast 1 and 143 mm for face Cast 2. Axial upward motion experienced at the offset location, due to butt curl, accounts for the differences observed between the two face locations. Both the morphological and transition position differences indicate that thermal
behave in is affected by ingot deformation during startup. It is believed that the significance of the coupling between temperature and deformation increases with magnitude of butt curl development or more generally, distance from the ingot center location.

In addition to surface topography, the severity/type of mould cooling also influences microstructure below the surface. The nature and severity of mould cooling in the lapped regime contributes to the formation of interlap discontinuities. These defects appear as cracks extending from the surface inwards in a direction roughly parallel to the advanced cooling heat flow. An example of an interlap discontinuity is shown in Figure 4.11. These defects can be considered as potential sites for subsequent crack generation. However, the interlap discontinuities occur in all casts, therefore their presence is not a sufficient criterion as a means of anticipating crack formation.

The lower cooling intensity associated with the exudated surface morphology creates a thermal condition suitable for inverse segregation of magnesium to the surface. A longitudinal section of the ingot, taken perpendicular to the surface, from near the center of the broad face was polished and then etched with sodium hydroxide. Analysis of the etched microstructure (Figure 4.12) reveals the presence of a magnesium enriched zone at the surface (darker region). EDX analysis has confirmed the presence of higher than nominal values of magnesium in this region. The thickness of the enriched zone was observed (Figure 4.12) to reach a maximum at a point approximately 50 mm above the transition before subsequently decreasing further up the casting. Based on our knowledge
of surface enrichment, this behaviour suggest that mould cooling intensity is at a minimum at this stage.

Figure 4.11  Interlap discontinuity.
Figure 4.12 Longitudinal cross section showing enriched magnesium layer at surface
5. Mathematical Models

In line with the goals of the research, a mathematical model capable of solving the governing heat conduction and deformation equations associated with both the inverse heat analysis and subsequent thermal stress simulation of the D.C. cast startup was needed. Toward this goal, a general finite element model developed by Cockcroft was adopted for the reasons outlined earlier.

5.1 Development of Mathematical Heat Flow Model

The purpose of this section will be to briefly review the application of the finite element method in solving the governing thermal heat conduction equations associated with our problem. As more detailed analyzes of the finite element method are presented in the literature, this review will focus only on the basic methodology required in solving a transient casting simulation. Inherent to the governing differential equations used in describing thermal behaviour, are material properties parameters such as thermal conductivity, density, latent heat and heat capacity. In the D.C. casting process these properties are necessarily a function of temperature and introduce an additional non-linearity into the system of equations. Thus, this review will encompass a synopsis of the techniques required to defining temperature dependent material properties in the FEM analysis. The values of the material properties will also be presented.
5.1.1 Formulation of Heat Transfer Problem

For the regions of the ingot being examined, a two-dimensional thermal heat transfer analysis was deemed sufficient, however, the nature of the problem ultimately requires a full three-dimensional model to adequately represent stress evolution. As the general techniques employed in analyzing both a two and three dimensional heat conduction problem are similar, for the purpose of expediency, only the three dimensional system will be discussed. The governing differential equation for heat conduction in three dimensions is:

\[
\frac{\delta}{\delta x} \left( k_x \frac{\delta T}{\delta x} \right) + \frac{\delta}{\delta y} \left( k_y \frac{\delta T}{\delta y} \right) + \frac{\delta}{\delta z} \left( k_z \frac{\delta T}{\delta z} \right) + Q - \rho C_p \frac{\delta T}{\delta t} = 0
\]  \hspace{1cm} (5.1)

with the boundary conditions of the form

\[ T = \Phi(x, y, z, t) \text{ on surface } S_1, \text{ for } t > 0 \]  \hspace{1cm} (5.2)

and

\[ k_x \frac{\delta T}{\delta x} n_x + k_y \frac{\delta T}{\delta y} n_y + k_z \frac{\delta T}{\delta z} n_z + q(x, y, z, t) + h(x, y, z, t)T = 0 \]  \hspace{1cm} (5.3)

and with the initial conditions:

\[ T = T_0(x, y, z) \text{ in domain } \Omega, \text{ } t = 0 \]  \hspace{1cm} (5.4)
where $S_1$ and $S_2$ represent surfaces of an arbitrary domain $\Omega$ on which the boundary and initial conditions are applied. The terms $n_x$, $n_y$, and $n_z$ represent the directional cosines of the normals to the surface of the domain. For an isotropic material the thermal conductivity, $k$, is non-directional, hence the subscripts $x$, $y$ and $z$ associated with this variable can be removed from the equations. Equation (5.1) is solved by employing a finite element discretization of the spatial derivatives. The non-linear system of ordinary differential equations which results from this approach is then solved using a step-by-step recurrence technique.

5.1.1.1 Finite Element Discretization of the Spatial Derivatives

An essential component of the finite element method are the interpolating polynomials used to determine the temperature within the discretized domain. For the purpose of this work the temperature within an element is defined by the following relation:

$$T^*(x,y,z) = \sum_{i=1}^{n} N_i(x,y,z)T_i(t) \quad (5.5)$$

where, $N_i$ are the nodal interpolation functions and $n$ is the total number of nodes per element. To best describe temperature variation across an element quadratic interpolation functions are employed. The interpolation functions are 2nd order polynomials. Based on the Galerkin weighted residual method and application of the Equation (5.5) to the governing equation (5.1), the following system of elemental equations are obtained:
\[
C^* \frac{dT}{dt} + K^* T + f^* = 0
\] (5.6)

where

\[
K^*_{i,j} = \int_B B^T_k B_j dV + \int_{S_2} h_i N_i N_j dS_2
\] (5.7)

\[
C^*_k = \int_B N_i \rho C_p N_j dV
\] (5.8)

\[
f_i = \int_B Q N_i dV - \int_{S_2} N_j q_i dS_2 + \int_{S_2} N_j h_i T_{Amb} dS_2
\] (5.9)

The elemental K matrix, so-called stiffness matrix, is dependent on the B matrix values or more specifically, the divergence of the shape functions, and on the thermal conductivity, \( k \), of the material. The B matrix in two-dimensions is defined as follows:

\[
[B(x,y)] = \begin{bmatrix}
\frac{\partial N_1}{\partial x} & \frac{\partial N_2}{\partial x} & \cdots & \frac{\partial N_s}{\partial x} \\
\frac{\partial N_1}{\partial y} & \frac{\partial N_2}{\partial y} & \cdots & \frac{\partial N_s}{\partial y}
\end{bmatrix}
\] (5.10)

The elemental heat capacitance matrix \( C^* \) (Equation 5.8) contains the density and heat capacity properties and accounts for the sensible heat. The terms of the force vector \( (f_i) \) include; internal sources or sinks of heat \( (Q) \), applied heat transfer coefficients \( (h) \) and external sources or sinks of heat \( (q) \).
5.1.1.2 Solution Technique

To solve the heat conduction equation for the entire domain, it was necessary to assemble the elemental equation (Equation 5.6) into a global system of equations of the following form:

\[
C \frac{dT}{dt} + K T + f = 0
\]  

(Equation 5.11)

Equation 5.11 represents the simultaneous solution of all the elemental equations (Equation 5.6) in the domain. Because the equations are non-linear (time dependent), they must be solved using a time stepping procedure. The solution technique employed, uses a three point recurrence or Dupont scheme in which:

\[
\frac{K(T_{i+1} + T_{i-1})}{4} + \frac{C(T_{i+1} - T_{i-1})}{\Delta t_i} = f_i
\]  

(Equation 5.12)

where \( T_i \) represents the temperature at the \( i \text{th} \) time step. This equation requires the temperatures to be known at two successive time steps. Thus, for the first time step in the calculation a Crank-Nicholson was employed. This method requires only a knowledge of the initial temperature according to the following equation:

\[
\frac{K(T_i + T_{i+1})}{2} + \frac{C(T_i - T_{i-1})}{\Delta t_i} = f_i
\]  

(Equation 5.13)

Equation (5.12) can be arranged such that:
\[ AT_{i+1} = B \]  

(5.14)

The matrix A, has dimensions \( n \times n \), where \( n \) is the number of nodes in the entire system.

### 5.1.1.3 Element Type

The elements employed by Cockcroft\(^5\) are eight and twenty node (2D or 3D analysis respectively) isoparametric quadratic elements. An example of a twenty node element, in both the local coordinate system \((u,v,w)\) and the global coordinate system \((x,y,z)\), is shown in Figure 5.1. The important feature of this type of elements is the ability to handle distorted element shapes where the interpolation functions (Equation 5.5) are used to transform the local coordinate system to the global system. This capability allows for an element of arbitrary shape in the global system to be rectilinear with dimensions, \( u = -1,0,1 \), \( v = -1,0,1 \) and \( w = 1,0,-1 \) in the local system. For a more detailed discussion on the mathematical formulation of the eight and twenty-node quadratic isoparametric elements, the reader is referred to the appropriate text\(^56-57\).

![Figure 5.1 Twenty-node isoparametric quadratic element depicted in rectilinear form in local coordinate system \((u,v,w)\) and in global coordinate system \((x,y,z)\).](image)
5.1.1.4 Numerical Integration

A Gaussian Quadrature integration procedure was used to numerically integrate Equations 5.7 - 5.9 over the domain of the element. For numerical integration in three dimensions the following expression was applied:

\[ \int_{-1}^{1} \int_{-1}^{1} \int_{-1}^{1} f(u, v, w) \, du \, dv \, dw = \sum_{i=1}^{m} \sum_{j=1}^{m} \sum_{k=1}^{m} W_i W_j W_k f(u_i, v_j, w_k) \]  

(5.15)

where, \( W_i, W_j \) and \( W_k \) are the weighting coefficients at locations \( i, j \) and \( k \), respectively, and \( m \) is the number of integration points (Gauss points) within the domain of the element. For the purposes of this work, 3 x 3 (two dimensional) or 3 x 3 x 3 (three dimensional) Gauss integration points were considered, as opposed to the computationally more efficient (2x2) or (2x2x2). This integration scheme was adopted to enhance the calculation accuracy of the temperature dependent properties employed in the solution. For similar reasons, the force vector (Equation 5.9) in the 2 dimensional thermal simulation was integrated using five Gauss integration points along the surface. This was deemed necessary to accurately reflect the rapidly changing values of the temperature dependent heat transfer coefficient.

5.1.1.5 Latent Heat Evolution

An important aspect of modelling D.C. casting is the correct treatment of the latent heat of fusion released upon solidification of the molten aluminum. Numerically, the latent heat of transformation can be accounted for by one of three methods: 1) the distributed
heat source method; 2) direct modification of the heat capacity term or 3) adjustment to the heat capacity term based on the enthalpy method. In the first group, the release of latent heat is treated as a heat source term $Q$ (Equation 5.9). Unfortunately this method is prone to instability. In the second group, the heat capacity is artificially raised, over the liquidus-solidus temperature range, to account for the evolution of latent heat during this period. This procedure is more stable than the previous method as it is introduced through the C matrix term. However, the modification of heat capacity over a small temperature range (liquidus to solidus) during periods of large temperature change (in comparison to the liquidus-solidus temperature range) can result in individual gauss points missing the change in heat capacity associated with the release of latent heat. Thus, this heat would not be accounted for in the analysis.

The solution adopted modifies the heat capacity based on an average enthalpy and on temperature gradients within an element. This methodology is generally referred to as the Lemmon\(^{41}\) technique. This procedure gives a representative value of heat capacity while avoiding the possibility of missing the peak in the heat capacity equation. The resulting expression for the effective heat capacitance per unit volume in three dimensions is:

$$C_p^{\text{eff}} = \frac{\left(\frac{dH}{dx}\right)^2 + \left(\frac{dH}{dy}\right)^2 + \left(\frac{dH}{dz}\right)^2}{\left(\frac{dT}{dx}\right)^2 + \left(\frac{dT}{dy}\right)^2 + \left(\frac{dT}{dz}\right)^2}^{1/2}$$

(5.16)
5.1.1.6 Incorporation of Temperature Dependent Material Properties

The material property terms in the elemental integrals equations (Equations 5.6-5.9) are, to simplify the calculations, assumed constant when evaluating the integral. However, it is recognized that these thermophysical properties are temperature dependent. The procedure adopted evaluated the thermophysical properties at the Gauss point temperature within each element during numerical integration of the integrals. Other techniques, which employ an iteration scheme, such as the Newton-Raphson method were deemed impractical in view of the projected computational size of the problem.

To minimize the non-linearities in both the material properties and in the overall transient heat-flow formulation, a dynamic time stepping algorithm was incorporated. Based on the temperature behaviour in the previous two time steps, a value of $\Delta t$ (see Equation 5.12) would be set such that the maximum change in temperature, over the time step, could be controlled. This allows the material properties to be evaluated over relatively small temperature changes.

5.1.2 Verification of Thermal Model Formulation

The finite element formulation for thermal behaviour was verified by Cockcroft using analytical solutions for specific conditions. The verification problems included one-dimensional heat conduction with a heat transfer coefficient boundary condition and one-dimensional heat conduction with phase change. As the primary solver remains unchanged from Cockcroft’s work, reverification was deemed unnecessary.
5.1.3 Thermal Properties

The thermophysical properties adopted in the heat conduction problem, specifically conductivity, heat capacity, latent heat and density were obtained from the literature\textsuperscript{58-66}. For the latter three terms, a "rule of mixtures" (ROM) approach was used to calculate the properties, based on the composition of AA5182 as 95.5% Al and 4.5% Mg. The calculated specific heat ($C_p$) of the solid material is compared to a value\textsuperscript{36} obtained from direct measurements on AA5182 in Figure 5.2. The good correlation between the two curves indicates the suitability of the ROM method. A specific heat of 1097 J/kgK was used for the liquid. In the temperature range between the solidus (577°C) and liquidus (638°C), a linear interpolation technique was adopted to calculate specific heat. The $C_p$ correlation and the latent of heat of evolution of 397.1 KJ/kg were then utilized to determine the enthalpy equations required by the model. A summation of the equation used to describe the temperature dependent properties (specific heat, enthalpy and density) is given in Table 5.1.
Figure 5.2  Comparison of calculated specific heat vs. literature values.

At the initiation of research, there was a paucity of published temperature dependent thermal conductivity data for AA5182. Figure 5.3 graphs the measured conductivity data obtained from Logunov et al. \cite{60} for an Al - (4.8-5.8\%)Mg - (0.5-0.8\%)Mn alloy and the linear approximation of this data used in the FEM analysis. The room temperature value of 120 corresponds closely with the published room temperature conductivity of 123 W/mK\cite{39}. Included in the graph are the experimental conductivity curves for pure aluminum as determined by Logunov et al.\cite{60} and by Prasso et al.\cite{47} for AA5182. The large difference between the pure aluminum and the Al-Mg alloys indicates the sensitivity of conductivity to alloying addition. Though the conductivity data of Logunov and Prasso exhibit similar behaviour a 10\% difference in the absolute magnitude exists. The effects of this magnitude of variation in conductivity will be considered in the
subsequent analysis. The temperature dependent equations used for the conductivity in the model are presented in Table 5.1.

Table 5.1
Thermophysical Properties

<table>
<thead>
<tr>
<th>Variable</th>
<th>Temperature Range</th>
<th>Equation (T in °C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conductivity</td>
<td>$T &lt; 577$</td>
<td>$119.2 + 0.0623 \ T$</td>
</tr>
<tr>
<td>(W/mK)</td>
<td>$577 \leq T \leq 638$</td>
<td>$594 - 0.484 \ T - 0.00048 \ T^2$</td>
</tr>
<tr>
<td></td>
<td>$T &gt; 638$</td>
<td>$69 + 0.033 \ T$</td>
</tr>
<tr>
<td>Specific Heat</td>
<td>$T &lt; 577$</td>
<td>$897 + 0.452 \ T$</td>
</tr>
<tr>
<td>(J/kgK)</td>
<td>$577 \leq T \leq 638$</td>
<td>$-994.8 + 8 \ T - 0.0074 \ T^2$</td>
</tr>
<tr>
<td></td>
<td>$T &gt; 638$</td>
<td>1097</td>
</tr>
<tr>
<td>Density</td>
<td>$T &lt; 577$</td>
<td>$2647 - 0.194 \ T$</td>
</tr>
<tr>
<td>(kg/m³)</td>
<td>$577 \leq T \leq 638$</td>
<td>$3480 - 0.68 \ T - 0.0017 \ T^2$</td>
</tr>
<tr>
<td></td>
<td>$T &gt; 638$</td>
<td>$2559 - 0.297 \ T$</td>
</tr>
<tr>
<td>Enthalpy</td>
<td>$T &lt; 577$</td>
<td>$-22575 + 897.4 \ T + 0.226 \ T^2$</td>
</tr>
<tr>
<td>(J/K)</td>
<td>$577 \leq T \leq 638$</td>
<td>$-3.84 \times 10^6 + 7644 \ T$</td>
</tr>
<tr>
<td></td>
<td>$T &gt; 638$</td>
<td>$3.3664 \times 10^5 + 1097 \ T$</td>
</tr>
</tbody>
</table>
5.2 Development of Mathematical Thermal Stress Model

Like the FEM thermal model, the stress portion of the finite element code has already been developed. However, the procedure used was restricted to a time independent elastic solution. A more suitable formulation for the D.C. casting problem would include the effects of visco-elastic material flow at elevated temperatures. Thus, a methodology which allows the incorporation of non-recoverable deformation was necessary. Further, a three-dimensional stress analysis was needed. Inclusion of the entire body allows the effects of constrained thermal contraction to be considered on a global scale. Unfortunately, limitations on the computational capacity of the computer system employed restricted the quality of the three-dimensional stress analysis that could be
achieved. One manifestation of this constraint is that the thermal analysis and stress must be modelled uncoupled, whereby the effects of ingot deformation on thermal boundary conditions are not considered.

5.2.1 Formulation of Thermal Stress Problem

The methodology for solving elastic stress problems using finite elements has been well developed and therefore will not be discussed in great detail. The solution is based on simultaneously solving the set of governing differential equations for mechanical equilibrium (Equations 5.17-5.19) and the strain displacement relations for an elemental volume of elastic solid (5.20).

\[
\begin{align*}
\frac{\delta \sigma_x}{\delta x} + \frac{\delta \tau_{xy}}{\delta y} + \frac{\delta \tau_{xz}}{\delta z} + F_x &= 0 \\
\frac{\delta \sigma_y}{\delta y} + \frac{\delta \tau_{yx}}{\delta x} + \frac{\delta \tau_{yz}}{\delta z} + F_y &= 0 \\
\frac{\delta \sigma_z}{\delta z} + \frac{\delta \tau_{zx}}{\delta x} + \frac{\delta \tau_{yz}}{\delta y} + F_z &= 0 \\
\end{align*}
\]

\( \varepsilon = L u \) (5.20)

\( \sigma_x, \sigma_y \) and \( \sigma_z \) are the stresses (force per unit area) acting on planes with normals in the x, y and z directions respectively, \( \tau_{ij} \) is the shear stresses acting on a plane with normal i in the direction j, and \( F_x, F_y, \) and \( F_z \) are body forces acting in the x, y, and z directions.
respectively. In Equation (5.20), $\varepsilon$ is the strain vector, $u$ is the displacement vector and $L$ is the linear-operator matrix which relates displacement with strain. This equation is applicable for small deformations.

To make the problem tractable, the constitutive equations, used for describing the stress-strain relationships in an linear elastic solid, are included. The general form of the constitutive equation based on Hookes law are as follows:

$$\sigma = D(\varepsilon - \varepsilon_0) + \sigma_0 \quad (5.21)$$

where $\sigma$ is the stress, $\varepsilon$ the strain, $\varepsilon_0$ the initial strain, $\sigma_0$ the initial stress and $D$ the material property matrix calculated from the modulus of elasticity ($E$) and Poisson's ratio of the material. In a three dimensions global analysis, $D$ is a $6 \times 6$ matrix and each of the remaining vector terms, $6 \times 1$ column matrices. Based on the relations described above the principle of "minimum potential energy" was adopted as a solution methodology.

5.2.1.1 Finite Element Solution by the Displacement Method

The principle of minimum total potential energy can be stated as follows:

"out of all the possible displacements fields that satisfy the geometric boundary conditions, the one that also satisfies the equations of static equilibrium results in the minimum total potential energy of the body".
The total potential energy is defined as the sum of the internal potential energy (strain energy) and the external potential energy (external forces) that act on a system. To minimize the total potential energy, it is required that the first variation of the total potential energy be zero or more conveniently, the first variation in internal potential energy equals the first variation in external potential energy. As no external forces are being applied to the ingot during D.C. casting, the solution to the minimization of potential energy can be simplified to the following:

\[ \delta U_i = \int \nu (\delta \varepsilon)^T \sigma \partial V = 0 \]  

(5.22)

where \((\delta \varepsilon)^T\) represents the first variation of the strain. The integral shown is applied over the entire body, hence, the integration over the volume \(V\).

By applying the strain displacement relations (Equation 5.20) and the portions of the constitutive equation (Equation 5.21) applicable to D.C. casting (i.e. no \(\sigma_0\)) the following expression is obtained for defining deformation within each individual element:

\[ K' \{\delta\}' - f' = 0 \]  

(5.23)

For this equation the potential energy of the element is evaluated in terms of the nodal displacements \(u_i, v_i\) and \(w_i\) over the elemental domain. Quadratic interpolation functions were used to improve the accuracy displacement evaluation across an element. This leads to the following expression:
Based on these relationships, Equation (5.23) can be defined as

\[ K^*_{ij} = \int_{V^*} B^T_i D B_j \delta V \] (5.25)

\[ f^*_i = \int_{V^*} B^T_i D \{\varepsilon\} \delta V \] (5.26)

where, \( B \), the matrix of differential operators, is defined for two dimensional analysis by:

\[
B = \begin{bmatrix}
\frac{\partial N_1}{\partial x} & 0 & \frac{\partial N_2}{\partial x} & 0 & \cdots & \frac{\partial N_s}{\partial x} & 0 \\
0 & \frac{\partial N_1}{\partial y} & 0 & \frac{\partial N_2}{\partial y} & \cdots & 0 & \frac{\partial N_s}{\partial y} \\
\frac{\partial N_1}{\partial y} & \frac{\partial N_1}{\partial x} & \frac{\partial N_2}{\partial y} & \frac{\partial N_2}{\partial x} & \cdots & \frac{\partial N_s}{\partial y} & \frac{\partial N_s}{\partial x}
\end{bmatrix}
\] (5.27)

and \( N_i \) are the nodal shape functions.
For problems involving thermal stresses, differential thermal strain is accounted for by imposing a thermal load, identical to the initial strain ($\varepsilon_0$), such that force vector in equation 5.26 becomes the thermal force vector as follows:

$$f_{n}^{i} = \int_{V} B_{i}^{T} D \{ \varepsilon \}_{n}^{i} \delta V$$  \hspace{1cm} (5.28)

where, $\{ \varepsilon \}_{n}^{i}$ is the thermal strain vector at node $i$ and is defined as follows:

$$\{ \varepsilon \}_{n}^{i} = \begin{bmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \\ \gamma_{xy} \\ \gamma_{xz} \\ \gamma_{yz} \end{bmatrix} = \begin{bmatrix} \alpha \Delta T \\ \alpha \Delta T \\ \alpha \Delta T \\ 0 \\ 0 \\ 0 \end{bmatrix}$$  \hspace{1cm} (5.29)

where $\alpha$ is the thermal expansion coefficient and $\Delta T$ is the change in temperature measured from some datum.

5.2.1.2 Solution Technique

The elemental equations (Equation 5.23) are assembled into the following global system of equations:

$$K \{ \delta \} + f = 0$$  \hspace{1cm} (5.30)
to obtain a simultaneous solution for nodal displacements in the domain. The stress
distribution can then be calculated according to the following equation:

\[
\{\sigma\}_i = (B_i \{\delta\}_i - \{\varepsilon\}_n)D
\]  
(5.31)

where the elastic strain is the difference between the total strain as determined from the
nodal displacements and the imposed thermal strain.

5.2.1.3 Selection of Element Type

For the three dimensional stress analysis, a 20 node isoparametric quadratic
element was used. The order of the shape function is such that continuity of the
displacement field was maintained across all elements. Calculated from the first derivative
of the displacements, the resulting strain and hence, stress, varies linearly across the
element and is non-continuous at the element boundaries. To improve accuracy of the
stress calculations, strain was determined at each internal Gauss integration point and
linearly interpolated to the node positions. At nodes associated with more than one
element, the average strain at this node was determined.

5.2.1.4 Temperature Dependent Material Properties

Temperature dependent properties are incorporated into the solution by evaluating
the relevant mechanical properties at the Gauss point temperature within each element
during formation of the elemental matrices. The properties include the coefficient of
thermal expansion and the elastic modulus E. For the thermal expansion coefficient the
metal solidus (577 °C) was used as the datum, thus, the equation employed evaluates the total thermal strain undergone as the body was cooled from 577 °C to temperature T. The equation in the analysis was calculated from data obtained for pure aluminum. The thermal strain equation is presented in Table 5.2. The temperature dependent elastic modulus equation is also presented in Table 5.2. As with the thermal expansion coefficient, the elastic modulus data is for pure aluminum. Poisson's ratio was considered temperature independent and was fixed at 0.3.

Table 5.2
Temperature Dependent Mechanical Properties

<table>
<thead>
<tr>
<th>Variable</th>
<th>Temperature Range (°C)</th>
<th>Equation (T in °C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha\Delta T$ (^{62})</td>
<td>T &lt; 577</td>
<td>$-2.3493 \times 10^{-2} + 1.98 \times 10^{-5} T + 3.625 \times 10^{8} T^2$</td>
</tr>
<tr>
<td>Modulus (MPa) (^{63})</td>
<td>T &lt; 500</td>
<td>71600 - 31.35 $T$ - 3.452 $\times 10^2 T^2$</td>
</tr>
<tr>
<td></td>
<td>500 ≤ T ≤ 577</td>
<td>308945 - 523.5 $T$</td>
</tr>
<tr>
<td></td>
<td>577 ≤ T ≤ 638</td>
<td>72259 - 113.1</td>
</tr>
<tr>
<td></td>
<td>T &gt; 638</td>
<td>100</td>
</tr>
<tr>
<td>$v$</td>
<td>all temperatures</td>
<td>0.30</td>
</tr>
</tbody>
</table>

5.2.2 Incorporation of Deformation Strains

Permanent deformation can occur in D.C. casting as either time independent plastic flow or creep. Though both mechanisms of deformation are fundamentally distinct the
strain generated by either is indistinguishable and therefore can be included into the FEM model by a single parameter $\varepsilon_p$. Thomas et al.\textsuperscript{54} incorporated the deformation strain into the constitutive equation in a manner similar to the initial strain term $\varepsilon_0$ (Equation 5.21). The general form of the constitutive equation for both thermal contraction and non-recoverable deformation becomes:

$$
\sigma = D(\varepsilon - \varepsilon_r - \varepsilon_p) + \sigma_0
$$

(5.32)

Following through the solution technique described in the previous section, the elemental equation for minimization of potential energy that includes the effects of both thermal strain and non-recoverable deformation is as follows:

$$
K^* \left[ \delta \right]^* = f_T^* + f_p^*
$$

(5.33)

where

$$
f_p^* = \int_{V_r} B_i^T D(\varepsilon)_i \delta V
$$

(5.35)

5.2.2.1 Verification of Non Recoverable Deformation Technique

The results from a problem for which an analytical or exact solution was available were analyzed to verify the mathematical formulation of introducing non-recoverable deformation into the FEM model. The analytical solution describes the creep deformation of a beam subjected to a fixed temperature distribution and accompanying thermal strain.
A schematic of the problem is shown in Figure 5.4. The coordinate axis is orientated such that the x direction parallels the length of the body, the y direction is through the thickness and the depth corresponds to the z direction. Imposed on the beam is a temperature distribution calculated according to the following equation:

\[ T = -25 + 208.3x^2 \]  

(5.35)

Top and opposite bottom face have fixed nodal displacements in Y direction

Figure 5.4  Schematic of visco-elastic verification simulation.

The stress boundary conditions were set such that \( \sigma_y \) is non-zero and both \( \sigma_x \) and \( \sigma_z \) are zero. This was achieved by limiting the y displacement of the top and bottom surface nodes (as indicated in Figure 5.4) to zero and allowing free movement in the x and z directions by fixing the nodes along the centre plane of each of these directions. The
latter boundary conditions are shown in Figure 5.4 and are mirrored on the bottom surface. The initial analytical stress solution, based on an elastic modulus of $1 \times 10^5$ MPa, a thermal expansion coefficient of $2 \times 10^{-5}$ °C and Poisson’s ratio of 0.3, is:

$$\sigma_y = -E \alpha T = 50 - 416.6 x^2$$  \hspace{1cm} (5.36)

The stresses in the beam were then relaxed according to the following relation:

$$\varepsilon = 4.0 \times 10^6 \sigma$$  \hspace{1cm} (5.37)

Therefore the solution to the time dependent stress relaxation problem was:

$$\sigma_y = (50 - 416.6 x^2) e^{-0.004t}$$  \hspace{1cm} (5.38)

where $x$ is the location along the beam and $t$ is time in seconds.

Stress relaxation values for both the analytical solution and the FEM generated solutions, at two beam locations ($x = 0.2$ m and $x = 1.0$ m), are plotted in Figure 5.5 as a function of time. A calculation time step of 30 seconds was used in the FEM calculations. The reasonable fit between the analytical solution and the model verifies the correctness of the non-recoverable deformation calculation methodology incorporated into the FEM formulation.
Figure 5.5  Plot of stress vs. time for both the analytical and FEM calculations at two beam locations.
6. Inverse Heat Transfer Analysis

As stated in the objectives, the purpose of this work was to mathematically model the startup phase of a full size D.C. ingot. Essential to any modelling work are the inclusion of suitable boundary conditions. For the D.C. casting of aluminum, the key boundary condition is the surface heat flux in the direct chill water regime. As discussed in the literature, this boundary is best applied in the form of a surface temperature dependent heat flux which can be conveniently expressed as a system boiling curve. The calculation methodologies employed to obtain these curves were discussed in the literature review. However, owing to casting conditions prevalent during the startup, such as; two-dimensional heat flow, variations in casting speed, water flow rate and the spatial position of isotherms, an inverse heat transfer procedure directly applicable to the system being studied was not available. Therefore, a methodology for calculating the heat flux/surface temperature relations from cast-in thermocouple temperatures, was developed.

The inverse technique developed uses as input the data acquired from an embedded thermocouple and involves the successive application of a 1-D and 2-D finite element based heat conduction model. A key feature of the technique is its flexibility with regards to thermocouple location, changing casting speed and non-steady state conditions. A novel approach has been developed in which the initial thermal conditions for input to the two-dimensional analysis are determined by first conducting a one-dimensional inverse heat analysis.
6.1 One-Dimensional Inverse Heat Transfer Analysis

In the one-dimensional inverse heat transfer analysis, the surface flux is assumed to be solely a function of the temperature distribution normal to the surface. Along the broad faces of the ingot, this gives rise to a one-dimensional temperature distribution with one-fold symmetry as shown schematically in Figure 6.1. Given the ingot configuration adopted in the study, the domain of the analysis can be further reduced from 400mm to 200mm subject to the analysis being limited to only a short distance below the meniscus. The frame of reference employed in the one-dimensional heat flow analysis is Lagrangian (moving with the ingot) leading to a transient solution in which time is related to the position below the meniscus via the following relationship:

\[ y(t) = \int_0^t v(t) \, dt \]  \hspace{1cm} (6.1)

where, \( y(t) \) is the distance below the meniscus at a given time, \( t \), and \( v(t) \) is a time-dependent casting speed.

Using the finite element procedure described in Chapter 5, the one-dimensional heat conduction problem was solved subject to the following boundary conditions:

\[ T(x)|_{x=0} = T_s(t) \]  \hspace{1cm} (6.2)
\[-k \frac{dT}{dx} \bigg|_{z=200\,mm} = 0 \quad (6.3)\]

and initial condition

\[T(x)\bigg|_{t=0} = T_0 \quad (6.4)\]

where \(T_0\) is the pour temperature less some amount to account for loss of super heat.

**Figure 6.1** Transverse view of ingot half showing one-dimensional analysis plane.

An example solution to the one-dimensional problem is shown schematically in Figure 6.2, where \(T_{x,t}^{\text{FEM}}\) is the temperature at a distance \(x\) below the ingot face, or surface, at time \(t\) and \(T_{s,t}^{\text{FEM}}\) is the surface temperature at time \(t\). Also shown in the figure are \(T_{\text{TC1},t}^{m}\) and \(T_{\text{TC2},t}^{m}\), which refer to the temperatures as recorded by two embedded thermocouples.
located at arbitrary depths below the surface of the ingot. The subscript 1 refers to the thermocouple located closest to the surface and the subscript 2 refers to a second thermocouple, located at a greater depth. The rationale for adopting a time dependent Dirichlet boundary condition, Equation (6.2), rather than the more fundamentally correct Neuman convective boundary, is so that the driving force for heat flow in the ingot can be adjusted directly on the basis of a difference between a measured and predicted temperature.

![Figure 6.2 Schematic of temperature profile for one dimensional analysis at time t.](image)

Given the above description, a series of one-dimensional temperature distributions are determined commencing at $t=0$ by adjusting the surface temperature at the future time step, $T_{s,t+\Delta t}^{FEM}$, by an amount, $\Delta T_{s,t}^{FEM}$, according to the following equation:
The correction, $\Delta T_{s,i,t}^{FEM}$, is calculated based on the difference between the measured and predicted temperatures at the current time-step, as follows:

$$
\Delta T_{s,i,t}^{FEM} = R_{1-D} (T_{TC1,t}^{FEM} - T_{TC1,t}^{m})
$$

and is applied every fourth time step (application every fourth time step proved necessary to help compensate for the fact that the assumption of 1-D heat flow is poor). In Equation (6.6), $R_{1-D}$ is a relaxation factor, $T_{TC1,t}^{m}$ is the temperature measured with the embedded thermocouple, at the current time step, and $T_{TC1,t}^{FEM}$ is the temperature predicted by the FEM analysis at the location of the embedded thermocouple, at the current time step. Typically, the time step employed in the model is significantly smaller than the data acquisition rate used to acquire the thermocouple data, thus it is necessary to interpolate between the measured temperature values in order to calculate an approximate value for $T_{TC1,t}^{m}$. In the current analysis, a simple linear interpolation has been used.

The temperature distribution from the 1-D analysis is output at times, $t_i$, $i = 1,n$ where $n$ corresponds to the number of transverse nodal layers that comprise the mesh used in the 2-D inverse analysis. The times, $t_i$, are chosen so as to correspond to the axial position of the transverse nodal layers via Equation (6.1).
6.2 Two-Dimensional Inverse Heat Transfer Analysis.

The following assumption has been made in order to make the two-dimensional inverse problem tractable:

(1) The temperature distribution within the ingot relative to a frame of reference fixed with the mould does not change appreciably over the time required for a thermocouple to transit the two-dimensional cooling zone.

The consequence of this assumption, in terms of the current analysis, is that a single thermocouple moving through the region of interest can be used to establish a constant, time independent, axial temperature distribution at the location of the thermocouple from which a representative heat flux distribution can be extricated. The result is a series of measured temperatures, $T_{w_e,y_j}$, at various axial positions $y_j$, $j = 1,m$ where $m$ represented the number of data acquisition points. The axial positions $y_j$ will be dependent on the casting speed and data acquisition rate (refer to Equation (6.1)).

In the analysis, heat is assumed to flow normal to the ingot faces and axially, giving rise to a two-dimensional temperature distribution with one-fold symmetry; thus heat flow in only one-half of an axial plane oriented perpendicular to the broad face need be considered. A rectangular section 200mm in depth by 150mm in height, located as shown in Figure 6.3, has been employed as the domain of the 2-D analysis. As in the 1-D analysis, a depth of only 200mm is sufficient if the analysis is limited to only short
distances below the meniscus. The length of the domain, 150mm, was chosen to encompass the section of the ingot surface over which boiling heat transfer occurs. The frame of reference is again taken to be moving with the ingot and therefore, the temperature distribution sought is transient.

![Diagram](image)

Figure 6.3 Schematic of solution domain used for two-dimensional inverse heat calculation shown at $t=0$.

Based on the above description of the problem, and assuming isotropic behaviour, the two-dimensional heat conduction problem is solved by the finite element method subject to the following boundary conditions:
\[ T(x, y)|_{z=0} = T_s(t) \]  
(6.7)

\[ -k \frac{dT}{dx} \bigg|_{x=200\text{mm}} = 0 \]  
(6.8)

\[ -k \frac{dT}{dy} \bigg|_{y=0\text{mm}} = 0 \]  
(6.9)

\[ -k \frac{dT}{dy} \bigg|_{y=150\text{mm}} = 0 \]  
(6.10)

and initial condition

\[ T(x, y)|_{t=0} = T_0(x, y) \]  
(6.11)

The initial temperature distribution input to the two-dimensional analysis domain was calculated from the preliminary one-dimensional analysis as described above.

An approximation to the correct temperature distribution, and hence heat flux, is determined by seeking to minimize the difference between the measured and predicted thermal behaviour while moving the 2-D domain through the positionally fixed axial temperature profile obtained from the thermocouple measurement. In the two-dimensional inverse analysis this is achieved by simultaneously adjusting all of the surface temperatures \( T_{r_{x, y}}^{FEM}(t) (i = 1,n) \) within the domain of the analysis, where \( n \) corresponds to the number of surface nodes, or equivalently number of transverse layers on nodes that comprise the 2-D finite element mesh - refer to Figure (6.3). As will be demonstrated, the simulation
time required to approach a solution is relatively short, and hence, assumption (1) above is not compromised.

The surface temperatures at the current time step, $T^{FEM}_{s,y_i}(t)$, are modified by an amount $\Delta T^{FEM}_{s,y_i}(t)$ to yield the surface temperature at the future time step, $T^{FEM}_{s,y_i}(t+\Delta t)$, according to the following relationship:

$$T^{FEM}_{s,y_i}(t+\Delta t) = T^{FEM}_{s,y_i}(t) - \Delta T^{FEM}_{s,y_i}(t)$$  \hspace{1cm} (6.12)

The correction, $\Delta T^{FEM}_{s,y_i}(t)$, is calculated based on the difference between the measured and predicted temperature and rate of change in temperature at the current time-step, as follows

$$\Delta T^{FEM}_{s,y_i}(t) = R_{1,2-D}(t)[T^{FEM}_{TC1,y_i}(t) - T^{m}_{TC1,y_i}] - R_{2,2-D}(t)\left[\frac{dT^{FEM}_{TC1,y_i}}{dt}(t) - \frac{dT^{m}_{TC1,y_i}}{dt}\right]$$  \hspace{1cm} (6.13)

where, $R_{1,2-D}$ and $R_{2,2-D}$ are relaxation factors, $T^{m}_{TC1,y_i}$ is temperature measured with the embedded thermocouple at axial location $y_i$ and $T^{FEM}_{TC1,y_i}(t)$ is the temperature predicted by the model at time $t$, at axial location $y_i$, at the position of the thermocouple. As can be seen from Equation (6.13), if the difference between the predicted and measured temperature is positive, the surface temperature is decreased, whereas if the difference between the predicted and measured rate of change in temperature is positive, the surface temperature is increased. Application of this technique reveals that it is beneficial to weight the rate of
change in temperature term more heavily during the initial stages of the calculations and the absolute temperature term later in the calculations, hence the time dependencies shown in Equation (6.13).

The axial positions, \( y_i \), are updated at each time step based on Equation (6.1). As in the 1-D analysis, the time steps in the model will not necessarily result in integration times that yield axial positions \( y_i(t) \) which correspond to the positions of the measured temperatures, \( y_j \), thus it is necessary to linearly interpolate to calculate \( T_{in, i}^m \).

### 6.3 Verification of Inverse Heat Transfer Method

The transient two-dimensional inverse heat transfer model has been verified by using an finite element based model to simulate the behaviour of a hypothetical thermocouple embedded into an ingot, subject to a known surface heat flux profile. In the simulation model, heat is assumed to flow as in the two-dimensional inverse analysis. The domain of the analysis together with the idealized heat flux profile are shown schematically in Figure 6.4. The initial temperature of the body was set to 660 °C in order to reproduce the sensible heat present under actual casting conditions. The casting process is simulated by moving the two-dimensional analysis domain through the positionally fixed axial heat flux profile at a rate consistent with the withdrawal rate of an ingot (0.0009 m/s). The idealized heat flux profile is intended to reproduce the approximate heat flows in both the mold and direct chill regimes. The thermophysical properties used in the FEM simulation
were presented in Table 5.1. The boundary conditions and initial conditions for the simulation are presented in Table 6.1.

Figure 6.4  Schematic of inverse verification domain.
Table 6.1

Boundary conditions and solution for two dimension casting simulations.

<table>
<thead>
<tr>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Boundary Conditions</strong></td>
<td></td>
</tr>
<tr>
<td>Top Surface</td>
<td>$-k \frac{\partial T}{\partial y}_{y=\infty} = 0$</td>
</tr>
<tr>
<td>Bottom Surface</td>
<td>$-k \frac{\partial T}{\partial y}_{y=200,\text{mm}} = 0$</td>
</tr>
<tr>
<td>Vertical Centerline</td>
<td>$-k \frac{\partial T}{\partial x}_{x=200,\text{mm}} = 0$</td>
</tr>
<tr>
<td>Ingot Surface</td>
<td>$-k \frac{\partial T}{\partial x}_{x=0,\text{mm}} = q(y)$</td>
</tr>
<tr>
<td><strong>Solution Parameters</strong></td>
<td></td>
</tr>
<tr>
<td>time step</td>
<td>0.05 s</td>
</tr>
<tr>
<td><strong>Initial Conditions</strong></td>
<td></td>
</tr>
<tr>
<td>initial temperature</td>
<td>660°C</td>
</tr>
<tr>
<td>casting speed</td>
<td>0.0009 m/s</td>
</tr>
</tbody>
</table>

The surface temperature, $T_s$, together with the temperatures at the location of two hypothetical thermocouples, $T_{tc1}'$ and $T_{tc2}'$, were output from the simulation model every 3 seconds. The calculated surface temperature was used in conjunction with the applied axial heat flux profile to determine a boiling curve for the ingot. The hypothetical thermocouples were located at depths of 8mm and 25mm below the surface of the ingot,
at a height of 43 mm as illustrated in Figure 6.4. The output interval was adopted to simulate a reasonable data acquisition rate.

Once calculated, the model generated thermocouple data was used as the input to the one- and two-dimensional inverse heat transfer analyses in succession. In this manner it is possible to make a direct comparison between an applied, or known, heat flux distribution and one calculated on the basis of a thermal history measured with an embedded thermocouple.

6.3.1 One-Dimensional Analysis

Commencing first with the results of the one-dimensional analysis, the calculated cooling curve was compared to the applied cooling curve in Figure 6.5. The results shown were obtained using a relaxation factor, $R_{1-D}$, equal to 1/12. As expected, the calculated curve does not approach the applied curve until low surface temperatures where one-dimensional heat flow is approached. Figure 6.6 shows a comparison between the simulation thermocouple temperatures and the temperatures calculated from the one-dimensional inverse heat transfer analysis for values of $R_{1-D} = 1/4$, 1/12 and 1/48. At a values of $R_{1-D} = 1/4$, the temperature at TC2 is below the observed value indicating an overestimation of the near surface temperature gradient. Conversely a low relaxation factor ($R_{1-D} = 1/48$) would underestimate the near surface temperature gradient as the calculated TC2 is greater than hypothetical value. A $R_{1-D} = 1/12$ was deemed as a suitable balance between over and under estimating the near surface temperature gradients. The
sensitivity of the 2-D inverse method to the initial temperature distribution predicted by the 1-D analysis will be discussed later.

Figure 6.5  Comparison of applied boiling curve with predicted curve from 1-D analysis ($\bar{R}_{I,D} = 1/12$).

Figure 6.6  Comparison of hypothetical thermocouple temperatures at TC1 and TC2 with predicted values from 1-D inverse analysis for $R_{I,D} = 1/4$, $R_{I,D} = 1/12$ and $R_{I,D} = 1/48$. 
6.3.2 Two-Dimensional Analysis

The results of the two-dimensional inverse analysis, based on the initial 1-D temperature distribution ($R_{1-D} = 1/12$) are presented in Figure 6.7. This figure shows the calculated flux vs. temperature curves at inverse calculation times of 1, 6, 9 and 12 seconds (this calculation time refers to the elapsed process time and not to computational time). A relatively stable cooling curve was obtained by 12 seconds calculation time. This illustrates that convergence to a solution is readily obtained thus justifying our assumption of a constant heat flux distribution over the calculation time period. The relaxation factors, $R_{12-D}$ and $R_{22-D}$, used in the calculations are presented in Table 6.2 and were obtained by trial and error and represent an optimum between stability and time for convergence. The applied cooling curve is compared to the predicted cooling curve (at 12 seconds calculation time) in Figure 6.8. The agreement between the curves is good in both the transition and nucleate boiling regime, however in the vicinity of the peak flux (150°C) the calculated peak flux is approximately 10% too low. The oscillations observed in the transition portion of the calculated curve are believed to be related to the coarseness of mesh employed in the FEM analysis. The size of the domain employed in the inverse method is such that cooling curve calculation extends only to surface temperature of approximately 80 °C.
Figure 6.7  Development of calculated boiling curves as a function of calculation time (based on 1-D analysis of $R_{I,D} = 1/12$).

Figure 6.8  Comparison of predicted boiling curve (12 seconds calculation time) with applied boiling curve.
Table 6.2

Time dependent two-dimensional relaxation factors.

<table>
<thead>
<tr>
<th>Analysis calculation time (sec)</th>
<th>Relaxation value</th>
<th>Relaxation value</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$R_{1,2-D}$</td>
<td>$R_{2,2-D}$</td>
</tr>
<tr>
<td>0.0 ≤ t &lt; 0.5</td>
<td>1/32</td>
<td>1/16</td>
</tr>
<tr>
<td>0.5 ≤ t &lt; 1.0</td>
<td>1/32</td>
<td>1/12</td>
</tr>
<tr>
<td>1.0 ≤ t &lt; 2.0</td>
<td>1/32</td>
<td>1/8</td>
</tr>
<tr>
<td>2.0 ≤ t &lt; 4.0</td>
<td>1/16</td>
<td>1/4</td>
</tr>
<tr>
<td>4.0 ≤ t &lt; 8.0</td>
<td>1/12</td>
<td>1/2.2</td>
</tr>
<tr>
<td>t ≥ 8.0</td>
<td>1/8</td>
<td>1/1.4</td>
</tr>
</tbody>
</table>

To assess the correctness of the temperature distribution, the hypothetical thermocouple temperatures, $T'_{TC1}$ and $T'_{TC2}$, have been compared with the temperatures predicted from the inverse analysis in Figure 6.9. The results of this comparison indicate excellent agreement, not only at TC1, but more importantly at TC2. This is a crucial result as TC2 is not used in the inverse calculation and thus the comparison at TC2 is a good indicator of the veracity of the technique. To further explore potential sources of error, a comparison has also been made between the measured and predicted rate of change in temperature at the location of the hypothetical thermocouple TC1. These results are presented in Figure 6.10 and indicate that the inverse analysis slightly lags the hypothetical thermocouple data for times greater than about 60 seconds, which corresponds to the time at which peak rate of change in temperature is observed. This would appear to suggest that the inverse analysis fails to “keep up” with a rapidly changing temperature field which
may in turn result in error in the spatial distribution of the heat flux. However, based on
the results presented in Figure 6.8, the effect on the boiling curve would appear to be
small.

Figure 6.9 Comparison of hypothetical thermocouple temperatures at TC1 and TC2
with predicated values from 2-D inverse analysis.
Figure 6.10 Comparison of hypothetical thermocouple rates of temperature change at TC1 with predicted values from 2-D inverse analysis.

The effects of the initial 1-D temperature distribution on the form of the calculated cooling curve are illustrated in Figure 6.11. The cooling curves shown in this figure represent 2-D calculations using an 1-D temperature distribution calculated at $R_{I,D} = 1/4$, $R_{I,D} = 1/12$ and $R_{I,D} = 1/48$. The lowest relaxation factor ($R_{I,D} = 1/48$) exhibits the best approximation to the applied curve in the transition and peak regions but begins to deviate in the nucleate boiling regime. This would indicate that an overestimation of the gradient may reduce the amount of sensible heat available for extraction in the inverse model particularly in the vicinity of the peak flux. However, the absolute differences between the values are small, thus indicating that the 2-D inverse method is relatively insensitive to $R_{I,D}$. 
Finally, the sensitivity to thermocouple position has been examined by comparing the results for cases where TC1 is located at 6mm and 10mm below the ingot surface. The results, shown in Figure 6.11, indicate a relatively good fit to the applied boiling curve in both cases suggesting that the method will yield satisfactory results with thermocouples placed up to 10mm below the ingot surface. However, examination of the curves in the vicinity of the peak heat flux, reveals that there was a slight improvement for the case when the thermocouple was located nearest the surface. Overall, this result is consistent with expectation as one would anticipate a drop in resolution with increasing thermocouple depth.
6.4 Application of Inverse Method to Experimental Data

Having demonstrated the ability of the inverse method to calculate the cooling curve from a single thermocouple moving through a direct chill water regime, the technique can now be applied to experimental data with a reasonable degree of confidence. As described above, the inverse heat transfer analysis was based entirely on the thermal response of the near surface thermocouple, TC1, whereas the temperatures from the deeper thermocouple, TC2, are used only for verification purposes. As a consequence, thermocouples pairs in which the response of the near surface thermocouple was impaired, either due to lack of physical entrainment and/or electronic malfunctions, were not considered in the inverse analysis. The thermocouples that were deemed to have
performed adequately are listed in Table 6.3 (see Appendix A for full compilation). The location of each thermocouple pair has been described in the industrial measurement chapter. Included in the table, are the process conditions and surface morphology experienced by the thermocouple pair during the initial stages of direct water contact and also the measured distances of each thermocouple from the surface as determined from the post-cast autopsy of the ingots.

Table 6.3
Thermocouples to which the inverse analysis was applied.

<table>
<thead>
<tr>
<th>TC Pair</th>
<th>Cast #</th>
<th>Cast Velocity (mm/s)</th>
<th>Water Flow (l/s/m)</th>
<th>Surface Morphology</th>
<th>Position*</th>
</tr>
</thead>
<tbody>
<tr>
<td>Center - B 1</td>
<td>0.77 - 0.899</td>
<td>1.97</td>
<td>lapped</td>
<td>8.0</td>
<td>22.8</td>
</tr>
<tr>
<td>Center - T 1</td>
<td>0.899</td>
<td>3.33</td>
<td>exudated</td>
<td>12.5</td>
<td>28.5</td>
</tr>
<tr>
<td>Offset - M 1</td>
<td>0.899</td>
<td>1.97 - 3.33</td>
<td>transition</td>
<td>8.0</td>
<td>22.0</td>
</tr>
<tr>
<td>Offset - T 1</td>
<td>0.899</td>
<td>3.33</td>
<td>exudated</td>
<td>9.0</td>
<td>25.0</td>
</tr>
<tr>
<td>Center - B 2</td>
<td>0.77 - 0.899</td>
<td>1.97</td>
<td>lapped</td>
<td>9.0</td>
<td>20.0</td>
</tr>
<tr>
<td>Center - T 2</td>
<td>0.899</td>
<td>3.33</td>
<td>exudated</td>
<td>9.0</td>
<td>25.0</td>
</tr>
<tr>
<td>Offset - T 2</td>
<td>0.899</td>
<td>3.33</td>
<td>exudated</td>
<td>8.0</td>
<td>25.5</td>
</tr>
</tbody>
</table>

* distance from surface (mm)

Prior to the inverse analysis, a Savitzky-Golay smoothing technique was applied to all of the TC1 temperature values in order to remove any random noise (this was found necessary in achieving a stable inverse solution). This technique employs a least squares fit at a single temperature based on a fixed number of temperatures above and below this data.
point. For the purposes of this work a quadratic function was used as the local regression equation requiring 5 temperatures above and below the one of interest to be considered. The calculation parameters used in the smoothing operation are presented in Table B.1 (Appendix B). Typical thermocouple data (for Cast 2 - Center - T thermocouple) before and after smoothing is presented for comparison in Figure 6.13. As can be seen, the trend in the data is unaffected and only the localized fluctuations in temperature have been minimized.

![Figure 6.13](image)

Figure 6.13 Comparison of Cast 2 - Center - T raw TC1 temperature data with smoothed values.

The thermocouple data from the casting trials has been analyzed with the inverse heat transfer model described above. All the parameters input to the FEM conduction engine have been described earlier, including material properties for AA5182 (Table 5.1)
and the boundary conditions, initial conditions and model control variables presented in Table 6.1 with the exception of the ingot withdrawal rate. The ingot withdrawal rates utilized are those taken from the actual casting and are presented in Table 6.3 for each thermocouple pair. The parameters pertaining to the inverse model employed in the analysis are identical to those discussed above with $R_{I,D} = 1/12$ and the two dimensional relaxation factors as presented in Table 6.2.

6.4.1 Inverse calculations for Cast 2 - Center -T thermocouple pair

For the sake of expediency, only the thermocouple pair positioned at the center of the ingot and in the T location (Cast 2 - Centre -T) was analyzed in detail with regards to verification and error assessment. This would include comparisons between measured temperature and rate of temperature change with the values predicted from the inverse analysis.

6.4.1.1 Verification and Error Assessment

To begin, the inverse analysis must first predict correctly the temperature distribution in the casting in order to evaluate the temperature gradient at the ingot surface and subsequently the heat flux. To verify this aspect of the inverse calculation, the temperatures predicted by the inverse model for the reference thermocouple pair are compared with the measured temperatures in Figure 6.14 (except where noted all inverse calculations presented will be at calculation times of 12 seconds). As indicated previously, only the data from the thermocouple located closest to the surface is input to the inverse
analysis; thus the second thermocouple provides a means of independently assessing the inverse analysis. As can be seen, the results, indicate good quantitative agreement for the thermocouple located nearest the ingot surface, TC1, however the agreement with the second thermocouple located at greater depth, TC2 is not as good as expected. This difference may be partially attributed to both the error associated with the thermophysical properties and/or differences in axial positioning of TC2 relative to TC1.

Figure 6.14  Comparison of measured temperatures for TC1 and TC2 at Cast 2 - Center -T thermocouple pair with predicted values from inverse analysis.

Another important aspect of the inverse analysis is that it must also correctly predict rates of change in temperature in order to determine the axial distribution of heat flux. To this end, a comparison has been made between the predicted and measured rate of change in temperature, or cooling rate, at the location of TC1. The results of this
comparison are presented in Figure 6.15, which depicts the rate of change in temperature as a function of time, or equivalently, position below the meniscus. The bottom of the mould has been identified on the graph to aid interpretation. As can be seen, these results indicate good agreement particularly in the advanced cooling regime prior to water contact. At times greater than the peak in cooling rate the model predicted cooling rate slightly lags the measured value by up to 5 sec or 4.5 mm, given a nominal casting speed of 0.9 mm/sec.

![Comparison of measured rate of temperature change for TC1 at Cast 2 - Center - T location with predicted values from inverse analysis.](image)

Figure 6.15 Comparison of measured rate of temperature change for TC1 at Cast 2 - Center - T location with predicted values from inverse analysis.

Having achieved a measure of confidence in the model, it is now possible to shift focus to the predicted heat fluxes. The results of the inverse analysis proper are presented in Figure 6.16 which shows the surface heat flux (as a function of ingot surface...
temperature) attained after 12 seconds inverse analysis simulation time. On close inspection, there are several features of this plot which attest to its correctness. First, there is a clearly identifiable change in slope in the curve at around 100°C, which delineates the transition from nucleate boiling to convective cooling, and secondly, the basic shape is similar to that of the idealized curve (taken from the literature) shown in Figure 2.1. The various regimes in order of decreasing temperature are; transition boiling (525°C to 134°C), nucleate boiling (134°C to approximately 100°C) followed by convective cooling at lower temperatures. It should be noted that the calculated peak flux of 2.64 MW/m² is lower than that predicted by Bakken et al.22 which ranged from 4.0 to 5.6 MW/m², for a 1600 x 600 ingot. The reason for this difference is difficult to assess, but may be related to differences in water flow rate, surface morphology, water quality and/or alloy thermophysical properties employed in the calculation.

![Graph showing predicted flux vs. surface temperature curve using data from TC1 at Cast 2 - Center - T thermocouple pair.](image)

Figure 6.16 Predicted flux vs. surface temperature curve using data from TC1 at Cast 2 - Center - T thermocouple pair.
To assess the influence of altering the thermophysical properties of the alloy on the inverse results, the thermal conductivity used in the analysis was altered by ±10%. The results are presented in Figure 6.17 which compares the standard analysis with the computed values using a thermal conductivity ±10% of the equation given in Table 5.3. The difference in the curves indicates that the heat flux is sensitive to thermal conductivity, particularly in the transition and peak regions. Increasing the thermal conductivity by 10% results in an increase in the peak flux from 2.64 (134°C) to 2.82 (139 °C) MW/m². Similarly reducing the conductivity reduces the flux to 2.43 (132 °C) MW/m².

Figure 6.17 Comparison of calculated flux vs. surface temperature for a ±10% change in thermal conductivity.

Although each of the castings was autopsied to determine the location of the embedded thermocouples, it is reasonable to assume some error in this measurement.
associated with both the physical width of the thermocouple and the non-uniformity of the ingot surface. In order to assess the effect of this uncertainty on the calculated heat flux profile, the location of TC1 has been varied by ± 0.5 mm within the inverse analysis model. The results for TC1 depths of 8.5, 9.0 and 9.5 mm below the surface are presented in Figure 6.18 where 9.0 mm is the measure value. As can be seen from this figure, there are a number of features of the plot that are sensitive to thermocouple position including, the magnitude and temperature of the peak heat flux and the temperature of the transition from nucleate to convective cooling. For example, varying the position from 8.5 to 9.5 mm is observed to result in a decrease in the temperature of the peak flux from 142 °C to 122 °C, an increase in the peak flux from 2.57 MW/m² to 2.72 MW/m² and a decrease in the nucleate to convective transition temperature from 105°C to 91°C.

Figure 6.18 Comparison of calculated flux vs. surface temperature curves for TC1 at 8.5 mm, 9.0 mm and 9.5 mm using Cast 2 - Center - T thermocouple data.
In summary, based on the results of the verification and error assessment, it is apparent that the inverse model is able to analyze industrial data with only one major concern: that of precisely determining the position of the embedded thermocouple (under the assumption that the thermophysical data input to the model is correct). Fortunately, the transition from nucleate boiling to convective cooling, which occurs at the boiling point of water (100°C), can be utilized to "fine tune" the position of the TC1 thermocouple. Using this criteria, the location of TC1 for all thermocouple pairs analyzed was modified such that the transition described above occurred at the appropriate temperature. The resulting changes to all of the thermocouple positions have been summarized and are presented in Table 6.4.

It should be noted that for thermocouple pair Cast 1 - Center - T a reasonable adjustment to the position of TC1 position, to fit the thermocouple data to the nucleate boiling/convective cooling transition, was not possible (calculated cooling curve plotted in Figure B.* in Appendix B). Close inspection of the original TC data revealed anomalous behaviour in the rapid cooling portion (before the main peak) of the rate of temperature change vs. time data. The slight peak and plateau observed in this region of the temperature data could not be attributed to any physical phenomena. In view of the impact of this behaviour on subsequent evolution of heat transfer predicted by the inverse model, the data from the analysis of this thermocouple pair was not considered for further investigation.
Table 6.4
Modified TC1 thermocouples locations

<table>
<thead>
<tr>
<th>Thermocouple Pair</th>
<th>Corrected Distance from surface (mm)</th>
<th>Adjustment (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cast1-Offset-M</td>
<td>7.7</td>
<td>-0.3</td>
</tr>
<tr>
<td>Cast1-Offset-T</td>
<td>9.7</td>
<td>0.7</td>
</tr>
<tr>
<td>Cast1-Center-B</td>
<td>9.0</td>
<td>1.0</td>
</tr>
<tr>
<td>Cast2-Offset-T</td>
<td>7.6</td>
<td>-0.4</td>
</tr>
<tr>
<td>Cast2-Center-B</td>
<td>8.7</td>
<td>-0.3</td>
</tr>
<tr>
<td>Cast2-Center-T</td>
<td>8.9</td>
<td>-0.1</td>
</tr>
</tbody>
</table>

6.4.2 Analysis of the Casting Process

The results of the analysis of the remaining thermocouple data have been collated on the basis of vertical position in the casting (e.g. bottom (B), middle (M) and top (T)) in an attempt to delineate the effect of changes in the casting parameters and ingot surface morphology on heat transfer. The results are presented in Figures 6.19, 6.20 and 6.21 respectively. To help quantify the results, best fit lines have been drawn through each of the various cooling regimes - e.g. transitional boiling, nucleate boiling and convective cooling. The results of the analyses have proven difficult to interpret owing to a number of factors, thus the data is best discussed in light of the mechanisms that influence heat transfer to fluids.
Figure 6.19 Calculated flux vs. temperature data points for B thermocouple pairs and best fit lines.

Figure 6.20 Calculated flux vs. temperature data points for M thermocouple pair and best fit lines.
As seen in Figures 6.19-6.21, it proved necessary to employ two lines to represent the relation between heat flux and surface temperature in the transitional boiling regime. Mechanistically, it is reasonable to expect that the transition boiling behaviour, which combines aspects of both film and nucleate boiling, would develop with time and thus would in effect go through an initial transient before stabilizing at heat fluxes typical of the system boiling curve. The initial steep slope exhibited in the figures would represent the transient flux behaviour. The second shallower line is considered to represent the transition portion of the system boiling curve. Unfortunately, the absolute relations between flux and surface temperature shown for the transient region are dependent on the surface temperature at first water contact. As a consequence, there exists a unique relation describing the transient portion of the system boiling curve for every initial surface.
temperature. This problem is overcome by assuming a constant rate of change of flux with temperature in the transient region. Thus, at any initial water contact temperature the flux will evolve at a known rate with surface temperature until the relations dictating the characteristic portion of the cooling curve (or an extrapolation of it) are reached.

To determine any differences in the transition cooling regime that may arise due to changing process parameters, a comparison is made in Figure 6.22 between the lines fitted to the calculated cooling curves for the bottom (B), middle (M) and top (T) zones. One difference observed is that the maximum heat flux for the bottom zone (lapped surface morphology, low water flow rate and increasing casting speed) is higher than for the top region (liquated surface morphology, high water flow rate and high casting speed). At a glance, this is in contrast to what would be expected as the T zone is experiencing a higher water flow. However, it needs to be pointed out that the ingot surface has undergone a change from being lapped, or smooth, for the bottom thermocouple, to being liquated, or rough, for the top thermocouple. Based on a review of the relevant literature it is possible that the effect of these two differences could offset one another. Hence, it would appear that in this instance the increased surface roughness may be counteracting the influence of increased water flow leading to a net drop in peak heat transfer. In addition, it is also worth noting that the rate of change of flux with surface temperature in the transient portion is higher for the bottom zone compared with top zone. Presumably, surface roughness and/or water flow rate also play a role in the development of stable transient, transition boiling heat transfer.
The results of a comparison between the correlation's, for the bottom (B), middle (M) and top (T) zones, in the nucleate boiling regime, are presented in Figure 6.23. The results indicate that the top zone nucleate boiling line is shifted to lower temperatures relative to the curves based on data from the bottom and middle of the ingot. Mechanistically, a rougher surface would allow easier bubble nucleation, thus sustaining a more vigorous boiling (higher flux) to lower surface temperatures. A discernible difference also exists between the flux at which the transition from nucleate boiling to convective cooling occurs. At high water flow rate and rough surface (top zone) the transition occurs at $1.5 \times 10^6$ W/m$^2$ whereas, for low water flow rate and smooth surface (bottom zone) the transition occurs at approximately $1.0 \times 10^6$ W/m$^2$. These results are
consistent with other studies that have shown the convective transition heat flow to be proportional to water flow rate.\textsuperscript{9,13}

![Diagram of fitted lines in nucleate boiling region for the B, M and T zones.](image)

Figure 6.23 Comparison of fitted lines in nucleate boiling region for the B, M and T zones.

Finally, a comparison of the system boiling curves from the same locations in the two casting has been made in order to assess the influence of water temperature. The B zone thermocouple pair results, shown in Figure 6.19, indicate that the peak flux was slightly greater for the Cast 2 ($T_{\text{water}} = 19.4^\circ\text{C}$) vs. the colder Cast 1 ($T_{\text{water}} = 8.8^\circ\text{C}$). This trend is opposite to what would be anticipated based on other investigations in the literature\textsuperscript{6,11}, albeit these studies were conducted at much lower levels of subcooling. Due to oscillations in the vicinity of the peak, it was not possible to analyze the effects of water temperature in the T region.
The analysis conducted above has focused primarily on the behaviour of the B and T regions. Discussion of the heat flux/surface temperature relation observed in the M zone is limited due to the lack of thermocouple data (i.e. only one curve could be calculated for this zone) and because of the transient conditions, changing of both the water flow and surface morphology, prevalent in this region. However, the cooling curve calculated for the M region does bear a close resemblance to the B and T curves suggesting that conditions are not dramatically altered in this region.

In summary, combining the results of the inverse analysis, it is possible to develop two system boiling curves to describe the variation of heat flux with surface temperature during startup; one applicable for conditions of low water flow and a lapped surface morphology (B zone, Figure 6.19), and the other for high water flow rate and an exuded surface (T zone, Figure 6.21). The trends observed are for the most part consistent with the literature and with a mechanistic understanding of the factors that influence the transfer of heat to fluids. The one notable exception is with respect to the influence of water temperature.
7. Modelling Analysis of Startup Phase

In the previous section, the direct chill water heat transfer relations prevalent during the startup phase were determined. Based on these correlation's, it was possible to conduct a series of FEM simulations to analyze temperature, and ultimately stress behaviour in the lower portion of the casting. The first step in the analysis methodology was to determine the veracity of the heat transfer correlation's (as determined using the inverse heat model) by comparing the temperatures predicted by the model with the measured values. It was originally intended to proceed directly to a three-dimensional thermal simulation for the verification analysis and then input the calculated temperature data directly into an uncoupled stress analysis in order to quantify the development of tensile stresses as a function of the imposed thermal conditions. However, the magnitude of the problem, coupled with the computational restrictions imposed by the computer hardware necessitated the utilization of a relatively coarse element mesh which had the effect of appreciably decreasing the accuracy of the stress solution. As a consequence, the results of the stress analysis were at best only qualitative. Nevertheless, they serve to enhance our knowledge of stress development within the ingot during startup.

Given the limitation described above, the focus of the work was shifted to analyzing the evolution of temperature in the ingot with the aim of determining thermal conditions that may enhance the propensity for cracking. Based on a knowledge of the factors that influence the development of stress, both the rate of temperature change at the
surface and the shell thickness immediately below the mould were considered as important thermal indicators. From the results of the investigation, casting variables, such as water cooling intensity and casting speed profiles, were adjusted as a means of modifying these indicators.

Having shifted the investigations of stress development to one based on heat-flow, the analysis portion of the study was undertaken employing a two dimensional model. The two-dimensional simulation was deemed suitable as heat flow at the centre of the broad face of the ingot, where cracking occurs, was two-dimensional (see discussion in the chapter on Industrial measurements). By limiting the analysis to two dimensions, it was practical to employ a relatively fine element size in meshing the region of interest, thus increasing the accuracy of the simulation.

7.1 Thermal Analysis

The thermal simulation was performed on a two-dimensional representation of an axial slice at the center of the broad face of the ingot. The heat transfer boundary conditions for the direct chill water cooling were calculated in the chapter on Inverse Heat Calculations. The heat transfer coefficients for cooling due to both the mould and starting block were gleaned from the literature\textsuperscript{25,26}. The thermophysical properties employed in the simulation have been presented in Table 5.1. The casting conditions (cast velocity profile) were presented in Table 4.1. The fill rate of the metal in the starting block until casting platform motion began was 1.1 mm/s. An initial metal temperature of 660 °C was
imposed. This value reflects the trough metal temperature minus a loss of some superheat as determined from thermocouple temperatures. To ensure calculation stability and accuracy an optimization routine was employed to dynamically modify the simulation time step to ensure that the maximum change in temperature in the body over a time step was 10 °C.

7.1.1 Boundary Conditions

A schematic of the two-dimensional simulation domain is shown in Figure 7.1. Included in the schematic is the position of the mould (at an arbitrary time), the point at which the direct chill water is imposed and the liquid metal level. Application of both the direct chill water boundary conditions and mould cooling are referenced from the liquid metal level in the simulation. As in the real casting system, the metal level, relative to the bottom of the ingot, is continually increasing as dictated initially by the fill rate of the starting block and then by the ingot casting rate. The faces or boundaries of the simulation subjected to both mould and direct chill water cooling are labeled as “DW (direct water)”. The surfaces which are exposed only to starting block cooling are labeled as “CC (contact cooling)”. The mesh employed for this domain consisted of 400 8-node isoparametric elements resulting in a total of 1283 nodes. A schematic of the mesh used is shown in Figure B.1 in Appendix B.
Figure 7.1  Schematic of domain employed in 2-Dimensional thermal simulation.

A listing of all the heat transfer boundary conditions employed in the thermal simulations are presented in Tables B.1 - B.4 in Appendix B. These tables furnish the equations used to describe the characteristic water cooling curves, the transient transition curves, mould cooling heat transfer coefficients and starting block cooling heat transfer coefficients. The specific heat transfer conditions were applied based on the axial position (y) in the ingot simulation domain relative to the metal level.
The equations describing the direct chill water heat transfer conditions (Table B.1) were calculated in the Inverse Heat Calculations section. It was determined that two system boiling curves were necessary to account for the changing surface morphology and water flow rate associated with the real casting. For illustrative purposes, the casting conditions at the Cast1 - Center thermocouple location are discussed. For this cast, the lapped surface morphology was observed to extend for 160mm above the ingot lip. In accordance with this measured value, the heat transfer conditions calculated for the lapped structure and low water flow (referred to as the B cooling curve in Table B.1) would be applied for the first 160 mm of ingot face. For axial locations along the ingot face in the simulation greater than 160 mm above the lip, the cooling curve equations would take the form calculated for the high water / exudated surface (referred to as the T cooling curve in Table B.1). It should be noted that the effect of changing water flow rate and the transition in surface morphology that occurs between the lapped and exudated regions is not considered in the analysis due to a lack of supporting data in this zone.

For both cooling curves, a minimum flux of 0.5E6 W/m² was imposed. Experience has shown that this minimum flux was required to prevent the surface temperature from becoming “stalled” at a particular value. It is believed that this minimum is necessary because the response of the thermocouple used in the Inverse Heat Calculations (located 8mm from the surface) is insufficient to enable the IHC calculations to accurately predict the instantaneous heat extraction as the water first contacts the ingot. The equations describing the transient transition portions of the cooling curves are presented in Table
B.2. The transient equations are employed until the transition portion of the characteristic cooling is reached.

The mould cooling boundary conditions are applied based on both the distance of the calculation point below the metal level and the observed surface morphology at this location in the casting. The equations describing mould cooling are summarized in Table B.3. In the regions of the ingot exhibiting a lapped surface morphology, a mould cooling heat transfer coefficient simulating a high rate of heat removal was applied for an interval along the ingot face in the range of 25 to 40 mm below the metal surface level. This range corresponds to the approximate width of a lap observed in the real casting at the center of the ingot. The value of the heat transfer coefficient (2500 W/m²°C) is consistent with theoretical studies on metal / mould contact cooling and with published modelling simulations in which heat transfer coefficients in the range 2000-4000 W/m²°C were employed to represent high intensity mould cooling. Along the remainder of the mould length, the severity of cooling was maintained at a relatively low value (Hc = 200 W/m²°C). This attempts to simulate the heat transfer conditions that are associated with a gap formation between the mould and the ingot. Similar values of heat transfer coefficient were used to simulate the transfer of heat from the bottom of the casting to the starting block. The heat transfer coefficient values for starting block cooling are listed in Table B.4.

Once above the lapped surface morphology (for Cast1 - Center of broad face this equals 160 mm), the heat transfer coefficient was maintained at 200 W/m²°C for the entire
length of mould cooling. In view of the exudated surface observed for this region, this seems like a reasonable approach. For all mould and starting block cooling heat transfer coefficients, the ambient temperature was set as 0°C.

7.1.2 Verification

For brevity only the results from the simulation of the Cast 1 - Center and Cast 1 - Offset (see Figure 4.1 for definition of Center and Offset thermocouple locations) conditions will be discussed. Additional comparison between predicted and measured temperatures are presented in Appendix B.

7.1.2.1 Center Thermocouple Locations

The results of the simulation for conditions at the Cast 1 - Center thermocouple location are compared to the measured values as a function of platform drop in Figures 7.2 to 7.4 for the B, M and T thermocouple pairs, respectively. To compensate for the upward displacement of the face due to butt curl, the platform values for the measured M and T thermocouples have been adjusted by 7 mm (subtracted). It should be noted that these adjustments are based on measurements taken of the final deformation after casting had been completed. No adjustment was made to the bottom thermocouple, as the amount of deformation that had occurred during its transit of the mould and initial portions of the direct chill water cooling regimes was deemed negligible. Subsequent stress analysis has validated this assumption.
Overall, the agreement between the measured values and predicted temperatures was reasonably good in both the mould and direct chill water cooling zones for the B and T thermocouple locations. The fit at the M location was not as good. In particular, the measured and observed temperature values are observed to deviate from each other in the region of rapid temperature drop (point of water contact). However, it should be noted the data logger was experiencing some form of electronic malfunction in recording of the M-TC1 values at this point in casting. In addition, imprecise knowledge of the water cooling curve in the M range (transient water flow and surface morphology) and the effects of ingot deformation on disruption of water flow, may also partially account for the differences observed. Generally, the results would indicate that the inverse heat derived cooling curves are representative of the conditions prevalent at the cast start for the center ingot locations.

The comparison of the calculated temperatures with the measured values from Cast 2 - Center thermocouples are presented in Figures B.2 - B.4 in Appendix B. The heat transfer conditions in this comparison are identical to those presented in Table B.1 - B.4 except the lapped surface morphology range is extended from 160 to 168 mm with an accompanying extension of both the direct contact mould cooling and the application of the B cooling curve. As with Cast 1, the measured temperatures at the M and T thermocouple locations have been adjusted by 7 mm to account for final ingot deformation.
Figure 7.2 Comparison of FEM data with measured values at Cast 1 - Center B location.

Figure 7.3 Comparison of FEM data with measured values at Cast 1 - Center M location.
7.1.2.2 Offset Thermocouple Location

The heat transfer boundary conditions presented in Tables B.1 - B.4 were suitable for accurately simulating the thermal behaviour at the center thermocouple locations. However, these exact conditions are not entirely applicable to the offset thermocouple locations. As presented in the chapter on industrial measurements, the lapped structure at the offset ingot location extends for 130 mm in Cast 1 and 143 mm in Cast 2 above the ingot lip. In addition, the typical lapped surface morphology observed at the ingot center location extends for only 50 mm above the lip at the offset positions before changing into a mixed surface morphology. It is believed that this mixed mode surface morphology represents cooling conditions bridging those occurring with the distinctive lapped surface and the exudated morphology. As a result, a heat transfer coefficient of 1350 W/m²°C was
used as the direct mould contact boundary condition for axial boundary locations ranging from 50mm above the face lip to the start of the exudated surface morphology at each offset location.

With regards to the systems boiling curves, the B zone equations in Table B.1 were applied for the first 130 mm along the face for the Cast1 - Offset simulation and for 143 mm in the Cast2 - Offset simulation. The T boiling curve equations were applied at axial locations above these respective values in each simulation. Unfortunately, as the thermal and stress models are decoupled, the effects of butt curl experienced at the offset thermocouple locations were not included in the analysis. All other simulation conditions were identical to those described for the center thermocouple locations described earlier.

The calculated temperatures from the Cast1 - Offset simulation was compared to the measured data as a function of platform drop in Figures 7.5 and 7.6 for the M and T thermocouple pairs. Both the measured temperatures at the M and T locations have been adjusted by 22 mm to reflect the final deformation observed at this location. The high rate of butt curl deformation was increasing rapidly at the casting time when the B thermocouple pair entered the water contact zone (see Figure 4.9), therefore an deformation adjustment was not possible and the results for this region are not included in the verification. The agreement between the measured and predicted temperatures were reasonable for the T zone but the simulation values for the M exhibited noticeably lower temperatures (at a given platform drop) than the measured values. This discrepancy may
be partially attributed to the unknown nature of the exact heat transfer coefficients in the quasi-lapped region extending from 50 mm to 130 mm.

The calculated temperatures from Cast 2 - Offset thermocouples are compared with the measured values (at M and T locations) in Figures B.4 and B.5 in Appendix B. The heat transfer conditions employed in this comparison have been discussed above. For this cast the measured M and T temperatures have been adjusted by 16 mm to account for the final measured deformation.

![Figure 7.5 Comparison of FEM data with measured values at Cast 1 - Offset M location](image)
7.1.3 Simulation Sensitivity

A study of the sensitivity of the predicted thermal behaviour to the imposed water cooling boundary conditions in the B (lapped surface morphology) zone of the ingot was carried out. This investigation addresses the significance of distinguishing the casting into two cooling regimes B and T. A simulation of the Cast 1 - Center conditions (see Figures 7.2 -7.4) was repeated except the T boiling curve was applied for the entire length of the casting. The calculated temperature values, at the B and M locations, from the modified heat boundary conditions (T boiling curve only) are compared to the calculated temperatures from the Cast 1 - Center simulation conducted earlier.
On analyzing the results, a slight difference was observed between the temperature values at both the B and M thermocouple locations. The difference in TC1 values at the point of rapidly changing temperature was equivalent to a shift of approximately 2-3 mm of platform drop. It remains to be determined what affect, if any, this has on the propensity for crack formation.

Figure 7.7  Comparison of FEM simulation temperatures at the B and M thermocouple groups for Cast1 - Center simulation using either the B cooling curve or the T curve in the B zone of the casting.

7.1.4 Analysis of Thermal Behaviour

The simulations conducted above confirm the veracity of the imposed heat transfer boundary conditions in adequately predicting the thermal behaviour during startup. It is now possible to analyze temperature evolution during this period with a reasonable degree
of confidence. In view of our interest in crack formation, the simulation analysis will focus on the conditions at the center thermocouple group locations. In addition, as behaviour from both casts at this location are comparable, the investigation was conducted based on the Cast 1 - Center conditions. Henceforward, the thermal behaviour calculated using the Cast 1 - Center parameters will be referred to as the “standard” conditions.

As this portion of the work will attempt to relate temperature evolution in the ingot with propensity for cracking, it is necessary to understand the genesis of thermal stresses. As discussed in the introduction, thermal stresses arise due to constraints imposed on thermal contraction. These constraints manifest themselves on both the local and global scale in D.C. casting, where a difference in temperature between the interior of the body and the surface and the resultant global contraction along the length of the ingot are simultaneously occurring. The severity of differential thermal contractions is related to the heat extracted by the direct chill water which in turn are a function of the surface temperature (in accordance with the boiling curve) and the prevailing casting conditions.

Based on our understanding of thermal stress generation it was believed that both shell thickness and the magnitude of the surface temperature gradient can influence thermal stresses within the ingot. The amount of solidified material present (or shell thickness) in the vicinity of maximum cooling may decrease the ingots ability to relax stresses by non-recoverable deformation. The resultant effect of shell thickness would be most apparent when considering the relaxation of global thermal constraints along the length of the ingot. In itself, an understanding of the amount of solidified material is an
insufficient criterion for implying conditions of high potential stress generation. A knowledge of the temperature gradient at the surface is also deemed necessary as it can provide insight into the thermal contraction mismatch occurring between the surface of ingot and the interior. Though differential thermal contraction would only be considered at a local level, the net effect would influence the global contraction discussed above. Hence, in a thermal study concerning potential stress generation, both shell thickness and surface temperature gradients must be considered concurrently.

### 7.1.4.1 Surface Temperature at Water Contact

As discussed above, the values of surface temperature at water contact are important as they influence the rate of heat extraction in accordance with the imposed water cooling curve. Within the context of the FEM simulation, these values were easily calculated. The variation in surface temperature at water contact (for the standard thermal simulation), as a function of cast length (cast length is defined as the length of the ingot face, above the lip, exposed to water cooling) is graphed in Figure 7.8. Included in the figure are arrows indicating the cast lengths (or equivalently casting times) that coincide with: 1) the cessation of high heat transfer mould cooling up near the meniscus (i.e. change from lapped to exudated surface morphology), 2) the attainment of the nominal casting speed and 3) the change in water cooling curves from the B shape to the T form. The pertinent features of this graph are the rapid drop in surface temperature when the ingot first enters the direct chill water, followed by a quasi steady state plateau and finally an increase in initial contact temperature until steady state conditions are approached. A
notable change in surface temperature coincides with the transition from the B cooling curve to the T relation. A less dramatic change in the surface temperature profile was observed to be associated with the end of high heat transfer mould cooling.

![Diagram showing surface temperature at water contact as a function of cast length.](image)

**Figure 7.8** Surface temperature at water contact as a function of cast length.

The values of surface temperature at water contact are important as they influence the subsequent rate of heat transfer in accordance with applied cooling curve. However, it was also necessary to consider thermal behaviour occurring within the ingot and how this behaviour (in particular shell thickness and surface temperature gradient) may influence the generation of stress.
7.1.4.2 Shell Thickness

In view of the importance of shell thickness, a method was developed to calculate the distance of the 577 °C isotherm (solidus temperature) perpendicular to the surface at an axial location parallel to the point of initial water contact. Though the effects of the solidified zone are two dimensional, a direct measurement of the shell thickness at the location indicated above allows this concept to be quantified. The calculated shell thickness, as a function of cast length (determined for the standard thermal simulation) are plotted in Figure 7.9. Included in the graph are arrows indicating the cast lengths (or equivalently, casting times) corresponding to: 1) the cessation of high heat transfer mould cooling at the meniscus and 2) the transition from the B to T cooling curves. Also included in the figure is a line indicating the cast length at which the butt curl rate measured in Cast 1 changes from a high rate of butt curl to a much lower value (see Figure 4.10). The rate of ingot deformation (butt curl) is an indication of the rate of stress relaxation, hence, the dotted line would also indicate a change from a high rate of stress relaxation to a much lower rate.
On examining Figure 7.9, a maximum shell thickness of 43 mm, at a cast length of 120 mm, was observed. The peak shell thickness at water contact region coincides with the approximate location at which cracking is observed to initiate (cracks are generally found to initiate in the vicinity of 150 mm above the ingot lip). The shell thickness was observed to decrease following the transition from the lapped to exudated surface and then level off as steady state conditions were approached. The shell thickness profile shown in Figure 7.9 exhibits a behaviour that is approximately the mirror image of the surface temperature graph shown in Figure 7.8. Thus, a minimum surface temperature corresponds to a maximum in shell thickness and vice versa, as would be expected.

Of additional significance, is the close correlation between the cessation of high heat transfer mould cooling (lapped surface) and the occurrence of both a maximum shell
thickness and a change in the rate of butt curl. This may indicate that the genesis of the lapped surface morphology occurring in the lower portion of the ingot is a function of both these phenomena. Intuitively, an increasing shell thickness would decrease the propensity for intensive mould cooling by enhancing the rigidity of the meniscus region. This would allow the ingot to structurally maintain a larger gap between the surface and the mould. As further evidence for this, a peak in the thickness of the enriched magnesium zone is observed at the surface following the transition (see Figure 4.12). This suggests reduced mould cooling through the formation of a larger gap and is consistent with the greater shell thickness in this portion of the casting enhancing structural rigidity. Subsequently, the enriched surface layer thickness decreases with increasing cast length in concert with a decrease in shell thickness.

### 7.1.4.3 Surface Temperature Gradient

A measure of the temperature gradient at the surface can provide a quantitative assessment of the thermal mismatch occurring between the surface and the interior. Within the FEM formulation, the temperature gradients in the axial and transverse direction at any surface location can be readily calculated. Based on these gradients, a resultant surface gradient can be determined in a manner analogous to calculating the resultant stress at a point from two orthogonal stresses. Figure 7.10 plots the resultant surface temperature gradients as a function of axial distance above the ingot lip, for two casting times equivalent to 100mm and 300 mm of cast length.
The 100 mm curve exhibits 2 peak surface gradients. The lesser peak corresponds to the rapid surface cooling associated with a high rate of heat transfer (exemplified by the lapped surface morphology at this cast length) within the mould/meniscus region. The more substantial peak arises from the intensive cooling imparted by the direct chill water. In terms of a comparison, the 100 mm curve exhibits a slightly higher peak gradient (24.2 °C/mm) at the surface than the 300 mm curve (21.2 °C/mm). In addition, by correlating the gradient with the calculated surface temperature it is observed that the peak gradient for the 100mm curve occurs at a surface temperature of 226 °C compared to 112°C for the 300mm curve. These differences may be partially attributed to variation in the shape, or form, of the cooling curves imposed in the simulation for the B and T regimes.

![Graph showing surface temperature gradients](image)

Figure 7.10 Surface temperature gradients as a function of distance above ingot lip for lengths of ingot exposed to cooling water of 100 mm and 300 mm.
The temperatures gradients at the same cast length shown in Figure 7.10, but calculated at a depth of 5 mm below the surface, are shown in Figure 7.11. Both curves exhibit a similar peak gradient (16.8 °C/mm), however, the magnitude of the temperature gradients at this location, are noticeably lower than the surface gradients (16.8 °C/mm as compared to 21.2 to 24.2 °C/mm). This suggests that the differences in the shape, or form, of the cooling curves applied in these simulations affect only the magnitude of the temperature gradients within 5 mm of the surface.

Figure 7.11 Resultant temperature gradients 5 mm below surface as a function of axial distance above ingot lip for cast lengths of 100 mm and 300 mm.

7.1.5 Thermal Behaviour Sensitivity

In the previous section, both shell thickness and surface temperature gradient were discussed as means of in-directly quantifying the potential for stress generation. Therefore
it is important that the sensitivity of these indicators to the imposed simulation cooling conditions be examined. The simulations executed in the sensitivity analysis were based on the Cast 1 - Center conditions as described earlier.

7.1.5.1 Sensitivity to Heat Flux/Surface Temperature Relation

The temperature data from the simulation in which the T boiling curve was applied for the entire cast length (see reference to Figure 7.7 : Section 7.1.3) was re-examined with the aim of determining the effects of curve shape on both shell thickness and surface temperature gradient. The observed shell thickness and the surface temperature gradients, at a cast time equivalent to 100mm of cast length were compared to the standard casting simulation (defined earlier) in Figures 7.12 and 7.13 respectively. Based on the comparison shown, the peak shell thickness was reduced slightly from 43 mm to 41 mm at an equivalent cast length. This result was expected given the lower flux values associated with the T boiling curve versus the B boiling curve.

In contrast, a more dramatic difference was observed with the resultant surface temperature gradients. As can be seen in Figure 7.13, the peak gradient was reduced from 24.2 °C/mm to 20.1 °C/mm by applying the T boiling curve for the entire cast length. The surface temperatures associated with the peak gradients locations were 226°C and 105°C for the standard and non-standard case, respectively. In addition, the peak temperature gradient for the modified simulation was shifted further down the ingot indicating that the lower fluxes associated with the transient portion of the T boiling curve are delaying the
attainment of the maximum flux. Overall, the results indicate that a small change in boiling curve shape has a significant effect on the resulting temperature distribution within the ingot primarily with regards to the surface temperature gradient and to a lesser extent the shell thickness.

![Graph showing shell thickness values](image)

**Figure 7.12** Comparison of shell thickness values from standard simulation with modified simulation (using only T cooling curve) as a function of cast length.
7.1.5.2 Sensitivity to Mould Cooling

The importance of mould cooling has been assessed by conducting a simulation using standard Cast 1 - Center conditions, except that the mould heat transfer coefficient associated with the lapped surface cooling was reduced from 2500 W/ m² °C to 1500 W/ m² °C, in the B region (see mould cooling equations in Table C.3). Both the shell thickness values and the surface temperature gradient at a casting time equivalent to a 100mm length of ingot exposed to water cooling are compared to the values obtained from the standard simulation in Figures 7.14 and 7.15 respectively. The shell thickness for the reduced mould cooling decreased from 43 mm to 38.5 mm at an equivalent cast
length. In addition, the shell thickness in the early portions of the casting were also significantly lower.

The peak surface gradient for the reduced mould cooling shown in Figure 7.15 was only slightly higher than the value observed with the standard simulation (24.8 °C/mm at 243 °C compared to 24.2 °C/mm at 226°C). The shapes of the gradient profiles are also very similar except in the meniscus cooling region. Overall the magnitude of mould cooling appears to have a significant influence over shell thickness. The attainment of a suitable shell thickness during the initial portion of the casting would then be strongly affected by the magnitude of heat extraction by the mould.

![Figure 7.14](image)  
*Figure 7.14* Comparison of shell thickness values from standard simulation with modified simulation (reduced mould cooling) as a function of cast length.
Figure 7.15 Comparison of resultant surface temperature gradients from standard simulation with modified simulation (reduced mould cooling) at a casting time equivalent to 100 mm of cast length.

7.1.6 Thermal Behaviour Optimization

The combination of maximum shell thickness, high surface temperature gradients and the reduction in the rate of butt curl may all have a bearing on thermal stress generation during startup. However, as mentioned earlier, the computational magnitude of the problem has limited our ability to quantify stress development, hence, our primary analysis was restricted to modifying the thermal conditions that may reduce the propensity for crack initiation. Based on our existing knowledge of thermal stress generation, the process may be optimized from the standpoint of cracking by reducing both the shell thickness and peak surface temperature gradient which in turn may be modified by manipulating either the cast velocity profile or the magnitude of direct water cooling.
Unfortunately, the effect of these parameters on ingot deformation (butt curl) and direct mould cooling cannot be considered in an uncoupled thermal analysis that would relate butt curl to gap formation. Thus, in the following optimizations, the extent and magnitude of mould cooling will be assumed to remain constant regardless of the casting process changes imposed.

7.1.6.1 Effect of Casting Speed

Though the absolute magnitude of the casting speed cannot be significantly altered without compromising either productivity and/or safety, the number of variations of casting profiles that can be imposed are limitless. To assess one possible scenario, the rate of increase from the initial casting speed to the nominal value was accelerated and started earlier. This was achieved by linearly ramping the casting speed from 0.72 mm/s to 0.89 mm/s in the platform drop span of 0 to 50 mm. In comparison, the cast velocity for standard simulation conditions is ramped from 0.72 mm/s to 0.89 mm/s in the platform drop span of 25 to 178 mm.

Figure 7.16 compares the shell thickness values, as a function of cast length, for both the standard cast velocity profile and the advanced casting velocity profile simulation. A maximum difference in shell thickness of 6.3 mm was observed between the two curves. This indicates that cast velocity has a significant effect on shell thickness. However, it is important to point out that the accelerated velocity simulation accounts only for the first order effect of changing the casting velocity profile on mould cooling (i.e. reduced
residence time in the mould). It fails to account for a second order effect and address the fact that a change to the temperature distribution within the ingot will result in a change in the gap profile or mould cooling profile. Unfortunately, only a fully coupled thermal mechanical analysis would permit exploration of this issue.

Figure 7.16 Comparison of shell thickness values from standard simulation with modified simulation (advance casting profile) as a function of cast length

Though the shell thickness was modified by altering the casting profile the resultant surface temperature gradients at the surface remained virtually unchanged. Figure 7.17 compares the gradients at a casting time equivalent to a cast length of 100mm. Except for a slight deviation in the region just below the peak (that amounts to an extension of the region of a higher flux), the temperature gradient curves for both
simulations are similar. The peak values were 24.7 °C/mm (at 248 °C) for the advanced casting profile and 24.2 °C/mm (226 °C) the standard simulation.

![Temperature Gradient Graph](image)

Figure 7.17 Comparison of surface temperature gradients from standard simulation simulation with modified simulation (advanced casting profile) at a casting time equivalent to 100 mm of cast length.

The simulation results exhibited above would indicate that the casting speed can be used to modify the amount of solidified material present in the vicinity of the water contact point but has a minimal influence on the surface gradients. However, the exact influence of casting speed is difficult to ascertain as its second order effects on mould cooling have not been accounted for.
7.1.6.2 Effect of Water Cooling Intensity

A second parameter that may be modified during the startup is the water flow rate. However, unlike manipulating the casting velocity profile, even the first order effect of reducing and/or increasing water flow is not known since the heat transfer correlation's do not exist. But, based on the trends observed in the literature, a reduction in water flow rate would result in a decrease in both the peak flux and the flux at the nucleate convective transition point for the system boiling curve. Thus, the effect of a qualitative decrease in water flow rate which would amount to a 10% reduction in heat transfer of the B boiling curve was simulated. The 10% reduction in flux was subtracted directly from the equations listed in Table B.1 for the B boiling curve.

The resulting shell thickness curves and surface gradients (at a casting time equivalent to a cast length 100mm) from the reduced B cooling simulation were compared to the standard condition values in Figures 7.18 and 7.19, respectively. The shell thickness was observed to be lower (difference in the peak region of 2.7 mm) for the reduced B boiling curve simulation. The reduced shell thickness extended for the duration of the application of the B boiling curve. As the same T boiling curve was applied in both simulations, the convergence of shell thickness at greater cast length was not surprising.

The peak surface temperature gradient (Figure 7-19) is observed to decrease from 24 °C/mm (226 °C) for the standard simulation to 21.7 °C/mm (259 °C) for the reduced cooling simulation. In addition, the reduced cooling data shows a slight shift in the
gradient to a position further down the ingot. The results indicate that a reduction in cooling water intensity can reduce the peak surface temperature gradients and to lesser degree the shell thickness.

![Figure 7.18](image_url)

Figure 7.18 Comparison of shell thickness values from standard simulation with modified simulation (B boiling curve reduce by 10%) as a function of cast length.
Figure 7.19 Comparison of surface temperature gradients from standard simulation simulation with modified simulation (B boiling curve reduced by 10%) at a casting time equivalent to 100 mm of cast length.

7.2 Stress Analysis

The development of thermal stresses in the D.C. casting process is exceedingly complex from both a practical point of view and also from a technical standpoint. The issue regarding the practical challenges - e.g. computational size of the problem with the resulting restrictions placed on mesh generation and the uncoupled formulation between thermal behaviour and stress development - have been alluded to previously. From a technical standpoint, the process involves large non-recoverable deformations occurring at high temperature combined with low temperature elastic plastic behaviour, the presence of extreme temperature gradients, the incremental addition of material and stress/strains
occurring in the mushy semi-solid material. In light of both these issues, the results of the stress are only exploratory, serving to inform as much as to yield insight into the development of stresses leading to surface face crack formation.

As will be demonstrated in the sections that follow, the results of the analysis are semi-quantitative in terms of their ability to predict macro-scale deformations (e.g. butt curl) and at best only qualitative in terms of the prediction of stresses. Unfortunately, owing to this limitation, it may be argued that the stress analysis does not contribute appreciably to our understanding of the development of stresses in D.C. casting. However, the considerable effort that has gone into the stress modelling has not been fruitless. The endeavour has yielded an understanding of the development of stresses in high temperature casting processes and an appreciation for the complexity of the problem. For this reason the analysis is included in the thesis.

To explore the development of stresses qualitatively, a three-dimensional thermal stress model of the D.C. casting process has been developed. As alluded to previously, the magnitude of the problem (physical dimensions of ingot) coupled with the computational limitations of the computer hardware available, imposed restrictions on the level of sophistication of the analysis. The restrictions were twofold; firstly, the size of the analysis domain necessitated a relatively coarse mesh; and secondly, the thermal simulation was conducted decoupled from the stress model. As a consequence, the modelling work will be presented in two sections; a thermal analysis section followed by the stress calculations.
7.2.1 Three Dimensional Thermal Model

In order to reduce the computational effort, conditions of symmetry have been applied with respect to heat flow parallel to the x and z directions within the ingot domain. With reference to the ingot schematic shown in Figure 7.20, a quarter section of the full size ingot was used as the domain in the analysis. This subdivision was based on conditions of symmetrical heat flow at the centerlines of the ingot. At these boundaries a condition of zero heat flow was specified such that for $t > 0$

$$q = -k \frac{\partial T}{\partial n} = 0$$

(7.1)

where $q$ is the flux, $k$ is the conductivity and $\frac{\partial T}{\partial n}$ is the temperature gradient normal to the surface. Along the faces of the ingot a temperature dependent flux was applied and was defined in a similar manner to Equation 7.2 except

$$q = -k \frac{\partial T}{\partial n} = f(T)$$

(7.2)

The adiabatic and applied surface flux boundaries conditions for a transverse slice of the ingot quarter section described in Figure 7.20 are shown in Figure 7.21.
Figure 7.20 Schematic of domain employed in 3-dimensional thermal simulation.
Figure 7.21 Schematic of transverse slice through 3-dimensional domain illustrating the flux boundary conditions.

In total, 1408 - 20 node isoparametric elements (6853 nodes) were utilized to fully mesh the analysis domain. To accommodate the ingot size being analyzed, it was found necessary to vary the dimensions of the elements with respect to both their axial and through thickness positions. Unfortunately the strategy employed resulted in relatively large elements in the upper portion of the mesh domain. The mesh employed is schematically shown, in Figures B.6 and B.7 in Appendix B, for a transverse slice and for an axial slice at the centerline parallel to the XY plane, respectively.

The exact casting parameters and cooling curves described in the thermal analysis section were employed in the three dimensional simulation. The effects of butt curl on the location and magnitude of both mould and direct water cooling were ignored. In addition,
the variation in the morphology and range of lapped zone (with resulting effect on heat transfer conditions) along the length of the ingot was not considered.

In total, four 3-dimensional thermal simulations were conducted. These are summarized in Table 7.2 below. The standard designation indicates standard Kaiser casting and cooling conditions applicable to Cast 1. The designation of H₂O bottom cooling indicates the effects of water entrainment beneath the ingot were considered in the thermal analysis.

Table 7.1
Summation of 3-Dimensional simulation conditions

<table>
<thead>
<tr>
<th>3D-simulation designation</th>
<th>Key Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>FEM1</td>
<td>standard run - no H₂O bottom cooling</td>
</tr>
<tr>
<td>FEM2</td>
<td>standard run - H₂O bottom cooling</td>
</tr>
<tr>
<td>FEM3</td>
<td>standard run - no H₂O bottom cooling, B cooling curve reduced by 10%</td>
</tr>
<tr>
<td>FEM4</td>
<td>standard run - no H₂O bottom cooling, cast velocity ramped from 0.72 mm/s to 0.899 mm/s over platform drop from 0 mm to 50 mm.</td>
</tr>
</tbody>
</table>

7.2.1.1 Standard 3D Thermal Simulation (no water entrainment)

The heat transfer coefficients applied to the portion of the domain representing the starting block are presented in Table B.3. As discussed earlier, these conditions attempt to reproduce the heat flux associated with initial contact cooling of the metal with the
starting block followed by the formation of an air gap. The ambient temperature was assumed to be 0 °C.

The predicted temperatures are compared to the measured values at the Cast1 - Center B and T positions and at the base thermocouples TC2, 7 (see Figure 4.3) in Figures 7.22, 7.23 and 7.24, respectively. The measured temperatures at the T location have been adjusted by 7 mm account for ingot deformation. The calculated thermal behaviour at the B and T thermocouple locations corresponds closely with the measured values, though the calculated temperatures exhibit slight deviations from the measure data. These deviations are attributed to the coarse mesh employed. The aberrations in the simulation data were amplified at the T thermocouple locations due to the gradual increase in element size with increasing cast length.

The agreement between measured and calculated temperatures in the ingot bottom (Figure 7.24) is not as acceptable as observed for the face thermocouples. The simulation temperatures calculated at the thermocouple position TC7 exhibited a similar trend to the measured values initially, but at casting times greater than 180 sec (direct chill water on ingot face and commencement of butt curl) the quality of the fit decreases due to a failure to account for heat transfer evolution in this portion of the casting. The calculated temperatures at the TC2 thermocouple location deviated substantially from the measured value following the commencement of butt curl. The greater difference observed at the TC2 thermocouple location emphasizes the significance of water entrainment beneath the ingot on cooling behaviour.
Figure 7.22 Comparison of 3-D simulation temperatures with measured values at Cast1 - Center B location.

Figure 7.23 Comparison of 3-D simulation temperatures with measured values at Cast1 - Center T location.
Figure 7.24 Comparison of 3-D simulation temperatures with no bottom water entrainment with measured values at the base thermocouple locations TC2 and TC7.

7.2.1.2 Standard 3D Thermal Simulation (water entrainment)

The simulation described above was repeated, except that cooling due to the entrainment of water between the ingot and the starting block was included. Based on the thermocouple data, measured butt curl and platform drop data (see Industrial Measurements) a relation by which the effects of water entrained cooling could be included in the thermal simulation was determined. The set of equations employed are presented in Table B.5 in Appendix B. These equations are based on the water entering beneath the ingot from the short ends where the distance of penetration of water cooling was calculated from the platform drop and the estimated butt curl. The flux used to simulate water cooling was fixed at 0.75 x 10^6 W/m^2. For casting times greater than 400
sec, this flux was reduced to $0.5 \times 10^6 \text{ W/m}^2$. Both these values were approximated from the fluxes derived from one dimensional inverse heat calculations with the bottom thermocouples.

The bottom thermocouple locations analyzed above (Figure 7.24) are compared to the simulation values in Figure 7.25. The TC7 location results remain the same as this location was not influenced by water entrainment, however a considerable improvement in correlation between the measured and calculated temperatures was achieved at the TC2 location. Though these results indicate the necessity of including the effects of water entrainment beneath the ingot, a large degree of uncertainty exists as to the extent and magnitude of this form of cooling. A more intensive experimental campaign would be required to fully understand this phenomenon. Subsequent stress analysis has shown, that for the conditions studied, inclusion of bottom cooling has a minimal influence on stress at the center of the long face. Therefore, given the uncertainty of the bottom heat transfer values, the remainder of the 3-dimensional thermal simulations were conducted without the inclusion of water entrainment. The results from the FEM-3 and FEM-4 simulations, were not elaborated on as the affect of the casting changes imposed in these simulations on thermal behaviour has been discussed earlier.
7.2.2 Three Dimensional Stress Model

As alluded to earlier, the analysis of thermal stresses in the D.C. casting process is both complex and numerically intensive. This complexity complicates the formulation of the stress model. To accurately simulate the generation of thermal stresses requires the incorporation of techniques to account for the continual formation of solid material and the wide variation in deformation mechanisms (creep, plastic flow and elastic) as the material is rapidly cooled. Unfortunately, the computational size of the problem necessitates the use of a relatively coarse mesh and a large time step. These simulation conditions compound the difficulties that arise when addressing the issues discussed above by eroding the numerical stability of the nonlinear stress problem. In an attempt to
counteract the consequences of a coarse mesh and large time step, several techniques and simplifications were employed. These techniques will be discussed briefly prior to presenting the results of the stress analysis.

7.2.2.1 Incremental Addition of Material

In order to predict stresses and deformations correctly, the model must attempt to account for the incremental addition of material to the ingot as it is formed and withdrawn from the mould. As the entire domain was premeshed, a “solid element criterion” was employed, whereby only elements possessing one node below the solidus temperature were included in the solution domain. However, the addition of elements in this manner results in a step change in the stiffness of the structure despite employing a low elastic moduli for the material in the elements being “switched on”. The effects of this step change in stiffness are amplified with increasing element size. On the positive side, the incremental addition of elements reduces the overall computational intensity of the problem.

To minimize the effect of incrementally adding elements, a methodology was implemented in which strains were added to the new solution elements such that the mismatch between the original mesh configuration and the deformed structure was reduced. For casting times when the metal level was above the starting block height, an initial strain component was added to each new layer of elements at or below the metal level. The calculated strains at the top surface of the element directly below the new
element were used as the initial strain values. These initial strains were added into the finite element calculations through the term $\varepsilon_0$ in Equation 5.21. A similar technique has been employed by others$^{48}$ as a means of ensuring continuity of the displacement and stress fields upon addition of new elements (the technique employed by Fjaer et al.$^{48}$ was based on the addition of strain to elements meeting the solidus criteria). The increment addition technique described above was observed to reduce the fluctuations in stress near the meniscus region and minimize any unrealistic deformation behaviour in this same region (i.e. ingot bulging).

During the initial stages of casting (metal level still within the starting block), a modified technique was employed. In this procedure, the thermal strains incurred in all the elements, currently in the analysis, were zeroed as each new layer of elements was added. This technique was incorporated to compensate for the combination of large elements and the exclusion of the presence of the starting block within this region of the casting - e.g. technique employed prevented unrealistic deformation (reverse butt curl) from occurring.

### 7.2.2.2 Deformation Behaviour

The total strain at any location within the ingot is a summation of the elastic, thermal and plastic strains that have occurred. With regards to the plastic strain term in the FEM formulation, the strains generated by either creep or visco-elastic deformation and/or time independent plastic flow or some combination of the two, are indistinguishable from each other. However, the methodologies used to determine the plastic strain occurring in a
calculation time step are very much temperature dependent, where the visco-elastic phenomena is prevalent at high temperatures and time independent flow predominated at low temperatures. To account for this difference, the non-recoverable deformation is calculated such that visco-elastic relaxation is assumed to occur at temperatures above 300 °C and time independent plastic flow below 300 °C. The 300°C limit stipulated was based on the deformation behaviour observed during high temperature compression testing. The subdivision of deformation behaviour based on temperature was implemented by Fjaer et al.⁴⁸ in their study of stress evolution within an AA6063 billet. In this study strain hardening was neglected at temperatures above 427 °C.

The Zener-Hollman equation⁶⁶ (Equation 7.4) was employed to determine the time dependent visco-elastic flow at high temperature. From this equation, the deformation strain rate a material would undergo, at temperature T and subjected to a stress σ, can be calculated. The parameters A, α and n, included in the equation, are material constants, Q is an activation energy term and R is the universal gas constant. Based on a series of high temperature compression tests⁶⁷ (300°C - 550°C) performed at a strain rate of 0.01/sec for AA5182, the values for A, α, n and Q were determined. These values are tabulated in Table B.6 in Appendix B.

\[ \dot{\varepsilon} = A (\sinh (\alpha \sigma))^n \exp \left( \frac{-Q}{RT} \right) \]  

(7.4)
Within a given time step the strain rate calculated via Equation (7.4) it is based on the current state of stress and temperature values. For small time steps its is reasonable to assume that neither of these parameters change appreciably. However, as the time step is increased, the assumption of a constant stress no longer holds true. As a result, the use of a reasonable time step (e.g. one yielding reasonable executable times) results in a significant overestimate in strain. This error stems from failing to properly address the reduction in stress occurring with strain (the process of stress relaxation).

In view of the relatively large time step employed in the analysis, a technique was developed such that the Zener-Hollman equation was numerically integrated according to the following expression:

\[ \Delta \varepsilon_p = \sum_{n=1}^{n_{lt}} \dot{\varepsilon}(t)(\sigma(t))\partial t(t) \]  

where \( t_1 \) is the initial time at the beginning of the time step, \( t_n \) is the final time at the end of the time step, \( \sigma(t) \) is the stress at a time \( t \), \( \dot{\varepsilon}(t) \) is the calculated strain rate at time \( t \) and \( \partial t(t) \) is the time integration substep. The deformation strain was obtained by evaluating Equation 7.5 over a number of \( \partial t(t) \) values such that the stress \( \sigma(t) \) was reevaluated at each \( \partial t(t) \) to reflect the reduction in stress that has occurred due to visco-elastic relaxation. The shortcoming of this approach is that it fails to preserve equilibrium as the global system of equations is not resolved at the end of subtime step. Despite this obvious
drawback, the technique yields a much better estimate of the strain occurring over a global
time step in the model.

For temperatures below 300 °C, a maximum allowable stress was imposed. Based
on the tensile test results of Horichuchi (Al-5%Mg alloy, conducted at a strain rate of
1.05x10^{-4}/s), an equation describing the maximum stress at any temperature was
determined. The maximum stress was defined as the UTS observed in the tensile tests. The
equations relating UTS with test temperature are presented in Table B.7 in Appendix B.

The maximum UTS (at any temperature) value described above is used as a means
of placing an upper bound on the stress occurring in any part of the ingot. This upper limit
is achieved by allowing plastic deformation to occur in the FEM calculations such that the
stress level would be relaxed to the UTS. The plastic deformation, over a time step, is
calculated from the following equation:

\[ \Delta e_p = \frac{\sigma - \sigma_{\text{max}}(T)}{E(T)} 0.5 \]  

(7.1)

where \( \Delta e_p \) is the plastic deformation occurring over the current time step, \( \sigma \) is the stress
from the previous time step, \( \sigma_{\text{max}}(T) \) is the UTS at temperature \( T \), \( E(T) \) is the temperature
dependent modulus and 0.5 is a relaxation factor. It should noted that this technique does
not consider the strain behaviour that would results prior to the attainment of the UTS.
The relaxation factor attempts to address the effects of global relaxation on the stress at
each calculation point. Overall, the imposition of a maximum stress results in more reasonable values of calculated stress.

To further lend stability to the solution, a maximum allowable strain, over a time step, was introduced. The levels of maximum allowable strain imposed are based on the location of the strain calculation position relative to the metal level. At the metal level the maximum allowable strain in an one second time step interval was 0.00067 and was linearly reduced to 0.000033 at distance of 50 mm below the metal level. The differentiation of maximum allowable strain accounts for the lower resistance to deformation of the material near solidus temperature. The maximum strains equations are listed in Table B.8 in appendix B. The imposition of a maximum strain within a time step minimized severe strain and hence, stress fluctuations in the body, thus reducing numerical instability.

7.2.2.3 Boundary Conditions

The stress analysis simulation did not consider any interaction between the ingot and either the mould or the starting block. The generation of stresses was based solely on the differential thermal contraction occurring. In addition, planes of symmetry, identical to those employed in the thermal model, have been adopted. Thus, only a quarter section of the ingot, as per Figure 7.20, is considered. At the planes of symmetry, the loads and forces were assumed to be equal and opposite. As a consequence displacements in the direction normal to these boundaries were set to zero. A schematic of a transverse slice
through the ingot (Figure 7.26) shows the fixed boundary conditions applied along the planes of symmetry. In addition, the displacement at a location in the ingot corresponding to the junction of the xy and zy planes and at an axial location, \( y = 0 \), was also set to zero. Because the effect of the starting block is not considered, this nodal constraint was required to suppress rigid body motion.

![Figure 7.26 Transverse slice showing stress simulation boundary conditions](image)

7.2.3 Stress Simulations

Using the temperature data from the thermal simulations listed in Table 7.2, a total of four stress simulations were performed. All simulations were conducted under identical simulation parameters. These included the material deformation characteristics described
above, the material properties, time step size and the inclusion of a maximum allowable strains. The calculation time step was set at 1 second.

7.2.3.1 Butt Curl Analysis

As a direct measurement of stress in the ingot during casting was not possible, the validity of the stress simulation was determined in part by comparing the calculated ingot deformations with the measured values. The axial displacement of the short end of the ingot predicted by the FEM analyzes was compared to the average measured values, from Cast 1 in Figure 7.27, as a function of cast length. The calculated deformations for all four stress simulations exhibited similar behaviour with respect to the measured values for cast lengths less than 80 mm. However, above this cast length, the calculated butt curl values began to deviate sharply from the measured data. The difference suggests that ingot rigidity was achieved more rapidly in the simulation than in the real casting thus limiting the magnitude of butt curl. Whether the enhanced rigidity was a consequence of thermal conditions, particularly with regards to starting block cooling or the lack of sophistication in calculating deformation strains at temperatures below 300 °C is not known.
Among the stress simulations themselves, the inclusion of water cooling along the ingot bottom resulted in the lowest overall butt curl. The "stiffening" of the ingot due to the additional cooling may account for the difference and would lend support to the assumption of enhanced rigidity influencing butt curl. For conditions of reduced heat extraction (FEM-3 and 4) the initiation of butt curl was delayed relative to the standard run (FEM-1). It is anticipated that the reduced heat flow per length of casting retarded thermal contraction and hence, delayed the development of stress and subsequent butt curl.

The axial deformations, calculated for the ingot lip at the center location, are graphed in Figure 7.28. Included in this figure is a line indicating the measured
deformation at this location at the termination of casting. Unlike butt curl, a greater difference is observed between the different analyses. The standard simulation (FEM-1) tends to overestimate the deformation in comparison to FEM-2 (water bottom cooling) which severely underestimates the final deformation.

Figure 7.28 Axial deformation observed at center of long face.

The results of the butt curl analysis indicate that the stress simulation gives a fair approximation to global deformation for the first 80 mm of cast length. This suggests that the stress analysis within this initial portion of the casting may be suitable for quantitative analysis. However, a reasonable approximation of butt curl values does not necessarily equate to the correctness of stresses calculated as butt curl deals with deformation on a macro scale and stress with strain on a micro scale. Therefore, a small error in the strain
calculated from the FEM model can equate to a relatively large error in the stress value. With these considerations in mind, the stress results were analyzed on the assumption that the data from the first 80 mm of cast length would be most representative of the real system.

7.2.3.2 Surface Stresses

Because of our interest in the propensity for stresses that may enhance cracking, only the development of $\sigma_z$ at the center of the long face of ingot was considered. Figures 7.29 and 7.30 compare the axial distribution of $\sigma_z$ along the ingot surface at casting times corresponding to cast lengths of 50 mm and 79 mm, respectively. In general, the stresses observed in the figures exhibit behaviour in agreement with the principles of differential thermal contraction. In both graphs, the maximum tensile stress occurred at an axial location below the water contact line. The relation of the peak location to the surface temperature gradient data will be discussed later. The magnitudes of the peak stress, 136 to 221 MPa for 50 mm cast length and 215 to 382 MPa for 79 mm of cast length, were considered reasonable given the UTS range of the AA5182 presented in Chapter 1 (276 to 421 MPa). It was also observed, following the attainment of a peak tensile values, that the stress gradually decreased and eventually near the bottom of the ingot face became compressive. The reversal in stress polarity results from the cool surface material being subjected to the thermal contractions of the interior material as it is cooled or perhaps the interior and exterior experienced different amounts of non-recoverable deformation. The reduction in heat extraction associated with both the reduced B cooling curve (FEM-3)
and the advanced casting velocity would result in a decrease in interior cooling and hence lower compressive stresses especially during the early stages of casting (Figure 7.29 - 50 min of cast length).

Figure 7-29  Simulation surffic stresses as a function of axial location at a cast length exposed of 50 mm.
Figure 7-30 Simulation surface stresses as a function of axial location at a cast length of 78 mm.

Unfortunately, it is difficult to directly compare the stresses observed from one simulation to the next due to the instability of the stress calculation. Figure 7.31 graphs the maximum stress $\sigma_{zz, \text{max}}$ along the face for FEM-1 (standard - no bottom cooling) as a function of length of ingot exposed to the direct chill water. The wide variation in stress observed precludes intra simulation analysis.
Figure 7-31 Maximum surface tensile stress ($\sigma_x$) observed for FEM-1 as a function of cast length.

However, it was possible to use the stress data to enhance our knowledge of thermal stress generation in D.C. casting. The variation in stress with axial location predicted for FEM-1 in Figure 7-30 is compared to the surface temperature gradients obtained from a comparable 2-dimensional thermal simulation in Figure 7-32. Both the surface stress and temperature gradient values were determined at a cast length of 79 mm. Given the coarseness of the 3-dimensional mesh, a very good correlation exists between the point of maximum stress and the peak surface temperature gradient. This data lends support to the hypothesis that the potential for cracking (resulting from a high tensile value of $\sigma_x$) is related to the surface temperature gradient.
Figure 7.32 Comparison of stress (FEM-1) and surface temperature gradient as a function of axial position at a cast length of 79 mm.

The affect of global ingot deformation (butt curl) on stress development at the center of the ingot was analyzed by comparing calculated butt curl with the maximum tensile stress observed for FEM-1. It was surprising to observe that the stress began to level off (general trend, not specific peaks and valleys) concurrent with the onset of similar behaviour in the butt curl. It was originally anticipated that stress would increase at the point of change in the butt curl as the accumulation of elastic strain energy, could not be relieved by this mechanism.
7.2.4 Summary

The results from the stress analysis indicate the difficulty of simulating stress evolution in large D.C. cast aluminum ingots. The combination of rapid heat extraction (variation in deformation behaviour) and nonlinear deformation behaviour requires the implementation of a small time step and fine mesh. However, due to computational restrictions, it proved necessary to utilize a relatively coarse mesh and large time step. Therefore several techniques were implemented that attempted to minimize numerical instability. Though the solution improved, the stress results were still ill-conditioned. As a consequence a quantitative assessment of stress evolution during casting startup was not possible, though a reasonable correlation was observed between temperature gradient and...
surface stresses. The inability of the stress model to accurately portray stress development necessitated a more detailed analysis of thermal conditions that may be conducive to crack generation.

Due to the 2-dimensional heat flow conditions prevalent at the center of the broad face, the thermal analysis was conducted using a 2-dimensional model. This avoids the problems associated with the large 3-dimensional mesh. The results indicate that both a variation in surface temperature gradient and in shell thickness are occurring during the startup phase of the casting. Based on our knowledge of thermal stress generation, these characteristics are believed to be important with regards to potentially detrimental stress development.
8. Summary and Conclusions

The work presented has entailed a comprehensive study of the starting process for a D.C. cast AA5182 rolling ingot. Mathematical models of heat flow and visco-elastic stress generation were employed to analyze this portion of the casting. The study included industrial measurements of ingot temperature and deformation behaviour during the startup period. In addition to model verification, the thermal data recorded was used as input to an inverse heat transfer model used in calculating the system boiling curves for the direct chill water.

The inverse heat transfer procedure developed for the study is capable of calculating a heat flux/surface temperature relation (system boiling curve) for the direct chill water regime. A distinct advantage of the inverse heat transfer technique is that a single thermocouple embedded within 8 mm of the surface and transiting the direct chill water regime can be employed to extricate the system boiling curve, thus relaxing the experimental constraints imposed by the necessity for the placement of multiple thermocouples near the surface. The formulation of the inverse heat technique includes the successive application of one-dimensional and two-dimensional FEM heat conduction models. Through the incorporation of these models the thermal behaviour of the thermocouple can be accurately simulated and the heat flux/surface temperature readily obtained.
The results of the inverse heat transfer calculations indicate that heat flows during the startup phase are complicated by changing ingot morphology and water flow rates. The water cooling intensity was found to be more severe in the “lapped surface morphology” region of the ingot though water flow rates were lower in this region relative to nominal water flow applied to the “exudated surface morphology” (remainder of the cast). For comparative purposes, the peak heat flux in the “lapped surface morphology” regime is 10% greater though the applied water flow rate is 45% lower. The differences were attributed to the effect of surface morphology on water boiling behaviour. These differences in ingot surface morphology are related to events occurring in the meniscus region within the mould. The lapped surface observed is indicative of a high degree of metal/mould contact resulting in a relatively high heat transfer. The occurrence of this surface morphology during the initial stages of casting are attributed in part to cast start procedures, mould design and metal flow to the meniscus region. Conversely, the exudated surface morphology prevalent for the remainder of the cast arises from conditions of minimal mould cooling.

A FEM simulation of the thermal behaviour at the cast start (based on the calculated system boiling curves) has indicated a correlation between a maximum in shell thickness and location of face cracking. A peak value in shell thickness (defined as the distance of the 577 °C isotherm from the surface at the point of water contact) of 43 mm was observed at a cast length of 125 mm. The magnitude of the shell thickness is related to both the severity of water and mould cooling associated with the “lapped surface
morphology" regime. In comparison the shell thickness decreased to 28 mm as steady state conditions were approached later in the casting. In addition, the peak surface temperature gradient was also observed to be higher within the "lapped surface morphology regime (25 °C/mm) than in the "exudated surface morphology" region (21 °C/mm).

Based on our knowledge of the process, the most expedient approach to influence startup conditions that may reduce the propensity for surface face cracking would be through the manipulation of the either the water cooling intensity and/or casting velocity profile. The review of the literature undertaken (see Chapter 2) indicates that water cooling intensity is proportional to water flow rate. Unfortunately, the limited casting conditions under which the thermocouple data was obtained does not allow direct quantification of the effect of a reduction in water flow on the intensity of water cooling (shape of the cooling curve) therefore only a qualitative reduction in cooling intensity was imposed. Based on the results of the reduced water cooling intensity FEM thermal simulation, a reduction in water flow rate during the critical cracking stages of casting would have a twofold effect: firstly, the shell thickness would be reduced and secondly, the peak temperature gradient at the surface would also decrease. A reduction in both these parameters is believed to reduce the propensity for cracking.

To circumvent potentially unsafe casting conditions, it is suggested that a reduction in water flow (from standard conditions) be implemented following 25 -50 mm of cast length. This would allow the shell thickness to reach a sufficient magnitude before
imposing a reduced cooling intensity. The water flow rate would then be increased once
the exudated surface morphology enters the direct chill water to account for the lessened
cooling intensity associated with this surface and the attainment of the nominal casting
speed. The current, or standard practice, of increasing water flow rate following 130 mm
of cast length may in actual fact be detrimental with regards to crack generation by
actually increasing cooling in the critical cracking zone.

The effect of advancing the start cast velocity profile (nominal casting speed
achieved after cast length of 50 mm as opposed to 150 mm) was analyzed in a FEM
simulation. The results indicates that an advanced casting velocity resulted in a reduction
in shell thickness of 6.3 mm. However, the magnitude of the peak surface temperature
gradient remained virtually unchanged. Given the influence of both this parameters on
stress development, it is believed that the manipulation of the casting velocity profile is a
secondary option as a means for modifying thermal conditions at the start that would
reduce stresses.

In view of the importance of surface morphology, a more long range approach to
minimize surface face cracking would be to control the cooling behaviour in the meniscus
region. The ability to minimize the occurrence or at least the severity of mould cooling
would be beneficial with regards to controlling the advent of the lapped surface
morphology. The effects of this meniscus control would be twofold: firstly, the
enhancement of heat extraction associated with the lapped surface morphology may be
minimized and secondly, the discontinuities between laps, which may act as potential crack
initiation sites, would be reduced. Unlike manipulation of the casting variables, control over meniscus cooling would require redesigning the mould system. For example, inclusion of a ceramic “hot top” casting system (used with aluminum billet casting) may be employed to alter heat flow patterns in this critical portion of the mould.

8.1 Recommendations for Future Work

The results of this research indicate that the D.C. casting system studied is relatively inflexible when it comes to the manipulation of thermal behaviour. The ability to alter thermal conditions through the manipulation of water flow rate and to a lesser extent casting velocity is limited. This suggests that a more fundamental understanding of conditions that can affect thermal behaviour (such as water jet design, water flow rate and external conditions such as surface morphology) is needed in the original design of the whole casting system. The design strategy would incorporate, as its foundation, an understanding of the fundamental heat flow conditions.

With the development of a sufficiently general inverse heat transfer methodology, our ability to study the relation between casting conditions and heat flow at cast start is enhanced. This research conducted to date has indicated surface morphology plays an important role in the heat flow conditions for the system analyzed. However, our knowledge of the influence of other casting parameters, such as water jet design, etc., is still minimal. In the long run, it is hoped that future work in D.C. casting modelling analysis will be aimed more to understanding the effect of these parameters on heat flow.
Based on this knowledge, it may be possible to design a casing systems for each alloy and ingot shape as opposed to primarily modifying the system (such as the cracking problem discussed here) after the fact.

With regards to the modelling portion of this work the conclusions drawn have been based primarily on the thermal behaviour occurring during startup. Unfortunately, the qualitative nature of the stress model could not be used to equate specific thermal conditions with specific stress levels, therefore a number of modifications to the stress model are needed. This would include; a more sophisticated approach to incorporating non-recoverable deformation into the simulation, a finer mesh to account for the wide variation in stress that can occur over a short distance and smaller time step to better reflect the scale of events occurring in the casting. In addition, the stress-strain-temperature data employed in any subsequent analysis would need to consider work hardening and the effects of changing temperature on this behaviour.
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Figure A.1  Transverse view schematic showing locations of base thermocouples from first casting trials.

Figure A.2  Measured temperatures vs. initial metal fill time from cast one (C1) base thermocouples.
Figure A.3  Measure temperatures vs. initial metal fill time from cast two (C2) base thermocouples.

Figure A.4  Measured temperatures vs. initial metal fill time for cast three base (C3) thermocouples.
Figure A.5  Temperature vs. platen drop time for the offset thermocouple group of face Cast 1.

Figure A.6  Temperature vs. platen drop time for the offset thermocouple group of face Cast 2.
Figure A.7  Temperature vs. platen drop time for the center thermocouple group of face Cast 2.

Figure A.8  Temperature vs. initial metal fill time for indicated base thermocouples locations from second casting trials. (refer to Figure 4.3 for details).
Figure A.9  Temperature vs. initial metal fill time for indicated base thermocouples locations from second casting trials (refer to Figure 4.3 for details).
Table A.1
Location of thermocouple of face groups from second casting trial measured perpendicular to surface (X) and above lip (Y).

<table>
<thead>
<tr>
<th>Cast Location</th>
<th>TC Group Designation</th>
<th>Axial Designation</th>
<th>TC1 X (mm)</th>
<th>TC1 Y (mm)</th>
<th>TC2 X (mm)</th>
<th>TC2 Y (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Offset</td>
<td>B</td>
<td>not entrained</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1 Offset</td>
<td>M</td>
<td>8.0</td>
<td>150</td>
<td>22</td>
<td>146</td>
<td></td>
</tr>
<tr>
<td>1 Offset</td>
<td>T</td>
<td>9</td>
<td>259</td>
<td>23.5</td>
<td>257</td>
<td></td>
</tr>
<tr>
<td>1 Centre</td>
<td>B</td>
<td>8</td>
<td>55</td>
<td>22.8</td>
<td>56</td>
<td></td>
</tr>
<tr>
<td>1 Centre</td>
<td>M</td>
<td>10.0*</td>
<td>148</td>
<td>24.5</td>
<td>152</td>
<td></td>
</tr>
<tr>
<td>1 Centre</td>
<td>T</td>
<td>12.5</td>
<td>242</td>
<td>28</td>
<td>242</td>
<td></td>
</tr>
<tr>
<td>2 Offset</td>
<td>B</td>
<td>not entrained</td>
<td>18</td>
<td>54</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 Offset</td>
<td>M</td>
<td>8.5*</td>
<td>150</td>
<td>23</td>
<td>150</td>
<td></td>
</tr>
<tr>
<td>2 Offset</td>
<td>T</td>
<td>8</td>
<td>247</td>
<td>25.5</td>
<td>245</td>
<td></td>
</tr>
<tr>
<td>2 Centre</td>
<td>B</td>
<td>8.7</td>
<td>47</td>
<td>20.0</td>
<td>47</td>
<td></td>
</tr>
<tr>
<td>2 Centre</td>
<td>M</td>
<td>not entrained</td>
<td>22</td>
<td>159</td>
<td></td>
<td></td>
</tr>
<tr>
<td>2 Centre</td>
<td>T</td>
<td>9</td>
<td>247</td>
<td>25</td>
<td>242</td>
<td></td>
</tr>
</tbody>
</table>

* electronic malfunction
Figure A.2
Location of thermocouples in base of ingot from second casting trial
(see Figure 4.3 for details).

<table>
<thead>
<tr>
<th>TC #</th>
<th>TC location</th>
<th>Distance from surface</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>transverse</td>
<td>longitudinal</td>
</tr>
<tr>
<td></td>
<td>(mm)</td>
<td>(mm)</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>508</td>
</tr>
<tr>
<td>2</td>
<td>0</td>
<td>508</td>
</tr>
<tr>
<td>3</td>
<td>0</td>
<td>381</td>
</tr>
<tr>
<td>4</td>
<td>0</td>
<td>381</td>
</tr>
<tr>
<td>5</td>
<td>300</td>
<td>228</td>
</tr>
<tr>
<td>6</td>
<td>300</td>
<td>228</td>
</tr>
<tr>
<td>7</td>
<td>300</td>
<td>0</td>
</tr>
<tr>
<td>8</td>
<td>300</td>
<td>0</td>
</tr>
<tr>
<td>9</td>
<td>0</td>
<td>254</td>
</tr>
<tr>
<td>10</td>
<td>0</td>
<td>254</td>
</tr>
<tr>
<td>11</td>
<td>165</td>
<td>450</td>
</tr>
<tr>
<td>12</td>
<td>189</td>
<td>228</td>
</tr>
</tbody>
</table>
Appendix B

Table B.1
Direct Chill Water Flux vs. Surface Temperature Relations.

<table>
<thead>
<tr>
<th>Temperature Range (°C)</th>
<th>Flux Equation (W/m² x 10⁶)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>B Zone:</strong></td>
<td></td>
</tr>
<tr>
<td>&gt; 550</td>
<td>0.5</td>
</tr>
<tr>
<td>550 ≥ T &gt; 367</td>
<td>3.290 - 0.004962 × T</td>
</tr>
<tr>
<td>367 ≥ T &gt; 139.3</td>
<td>3.756 - 0.006220 × T</td>
</tr>
<tr>
<td>139.3 ≥ T &gt; 116.2</td>
<td>2.890 - 0.0003561 × (T-139.3)^2</td>
</tr>
<tr>
<td>116.2 ≥ T &gt; 100</td>
<td>0.1047 × T - 9.476</td>
</tr>
<tr>
<td>≤ 100</td>
<td>0.253 + 0.007422 × T</td>
</tr>
<tr>
<td><strong>T Zone</strong></td>
<td></td>
</tr>
<tr>
<td>&gt; 550</td>
<td>0.5</td>
</tr>
<tr>
<td>550 ≥ T &gt; 367</td>
<td>3.290 - 0.004962 × T</td>
</tr>
<tr>
<td>367 ≥ T &gt; 135.2</td>
<td>3.294 - 0.004962 × T</td>
</tr>
<tr>
<td>135.2 ≥ T &gt; 103.8</td>
<td>2.624 - 0.0003631 × (T - 135.2)^2</td>
</tr>
<tr>
<td>103.8 ≥ T &gt; 99.6</td>
<td>0.2259547 × T - 21.09</td>
</tr>
<tr>
<td>≤ 99.6</td>
<td>0.026314 × T - 1.183</td>
</tr>
</tbody>
</table>

Table B.2
Transient Transition Equation

<table>
<thead>
<tr>
<th>Zone</th>
<th>Flux Equation (W/m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>B</td>
<td>0.5 + (T_{cont}** - T*) × 0.010543</td>
</tr>
<tr>
<td>T</td>
<td>0.5 + (T_{cont}** - T*) × 0.007658</td>
</tr>
</tbody>
</table>

* - surface temperature
** - surface temperature at initial water contact
Table B.3
Mould Cooling Heat Transfer Coefficients

<table>
<thead>
<tr>
<th>Distance below metal level (mm)</th>
<th>Hc for Lapped Zone (W/m²°C)*</th>
<th>Hc for Exudated Zone (W/m²°C)*</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 - 25</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>25 - 40</td>
<td>2500</td>
<td>200</td>
</tr>
<tr>
<td>40 - 70</td>
<td>200</td>
<td>200</td>
</tr>
</tbody>
</table>

*ambient temperature = 0 °C

Figure B.4
Starting Block heat transfer coefficients

<table>
<thead>
<tr>
<th>Distance below metal level (mm)</th>
<th>Heat Transfer Coefficient* (W/m²°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 - 5</td>
<td>0</td>
</tr>
<tr>
<td>5 - 10</td>
<td>2500</td>
</tr>
<tr>
<td>&gt; 10</td>
<td>200</td>
</tr>
</tbody>
</table>

* ambient temperature = 0 °C

Table B.5
Distance of water cooling entrainment beneath ingot

<table>
<thead>
<tr>
<th>Platform Drop (mm)</th>
<th>Butt Curl (mm)</th>
<th>Distance (from short end) of water entrainment (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>32 ≤ PD &lt; 180</td>
<td>-16 + 0.678 PD - 0.00175 PD²</td>
<td>-69 + 16.8 BC - 0.0792 BC²</td>
</tr>
<tr>
<td>PD ≥ 180</td>
<td>43 + 0.0341 * PD</td>
<td>-69 + 16.8 BC - 0.0792 BC²</td>
</tr>
</tbody>
</table>
Table B6
Constitutive equation (Zener-Hollman) parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>$8.9 \times 10^9$</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>0.039</td>
</tr>
<tr>
<td>$n$</td>
<td>1.77</td>
</tr>
<tr>
<td>$Q$</td>
<td>$-170000 \text{ J/mol}$</td>
</tr>
</tbody>
</table>

Table B7
Maximum Stress vs. Temperature Equation

<table>
<thead>
<tr>
<th>Temperature ($^\circ C$)</th>
<th>Maximum Stress (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$150 &lt; T \leq 300$</td>
<td>$70 + 0.98 \times (300 - T)$</td>
</tr>
<tr>
<td>$T \leq 150$</td>
<td>$326 - 0.00488 \times T^3$</td>
</tr>
</tbody>
</table>

Table B8
Maximum allowable strains

<table>
<thead>
<tr>
<th>Distance below metal level (mm)</th>
<th>Maximum allowable strain over 1 second calculation interval</th>
</tr>
</thead>
<tbody>
<tr>
<td>$0 - 50$</td>
<td>$\varepsilon_{\text{max}} = 0.00067 - [(Y_m^* - Y^{**}) \times 0.00033 / 50]$</td>
</tr>
<tr>
<td>$&gt; 50$</td>
<td>$\varepsilon_{\text{max}} = 0.00033$</td>
</tr>
</tbody>
</table>

$Y_m^*$ = axial position of metal level
$Y^{**}$ = axial position in ingot
all dimensions in mm

Figure B.1  Schematic of 2-dimensional simulation mesh.
Figure B.2  Comparison of FEM data with measured values at Cast 2 - Center B location.

Figure B.3  Comparison of FEM data with measured values at Cast 2 - Center M location.
Figure B.4  Comparison of FEM data with measured values at Cast 1 - Center T location.

Figure B.5  Comparison of FEM data with measured values at Cast 2 - Offset M location.
Figure B.6 Comparison of FEM data with measured values at Cast 1 - Offset T location.
Figure B.7  Schematic of transverse slice through 3-dimensional mesh.
Figure B.8 Schematic of axial slice through 3-dimensional mesh parallel to XY plane.

all dimensions in mm