A Boundary Condition Coupling Strategy for the Modeling of Metal Casting Processes

by

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A thesis submitted in conformity with the requirements for the degree of Doctor of Philosophy

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A Boundary Condition Coupling Strategy for the Modeling of Metal Casting Processes

Doctor of Philosophy, 1998

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Abstract

A generalized temperature boundary condition coupling strategy for the modeling of conventional casting processes was implemented via experiments and numerical simulations with cylindrical aluminum, aluminum alloy and tin specimens in copper, graphite and sand molds. This novel strategy related the heat transfer coefficient at the metal-mold interface to the following process variables: the size of the air gap which forms at the metal-mold interface, the roughness of the mold surface, the conductivity of the gas in the gap, and the thermo-physical properties of both the metal and mold. The objective of this study was to obtain, apply and evaluate the effect of incorporating an experimentally derived relationship for specifying transient heat transfer coefficients in a general conventional casting process.

A systematic experimental approach (not limited to a specific industrial process) was implemented to determine the heat transfer coefficient, and characterize the formation of the air gap at the metal-mold interface. The heat transfer mechanisms at the interface were identified, and seen to vary in magnitude during four distinct stages, as the air gap formed and grew. An semi-empirical inverse equation was used to characterize the heat transfer coefficient-air gap relationship, across the various stages, for experimental data from the literature and this study, and a correlation was presented in non-dimensional form for experimental data from this study.
The effect of surface roughness was observed to be pronounced at small relative gap sizes, reducing the heat transfer coefficient at least one order of magnitude below that predicted for perfectly flat surfaces. The effect was observed to progressively diminish with increasing gap sizes, and approached an analytical 'perfectly flat' solution for larger gap sizes.

A simplified visco-elastic plastic numerical model was developed for a cylindrical coordinate system to predict the growth of the air gap. The model's predictions of the gap growth compared well with the experimental measurements for each system examined. Application of the correlation via coupling with the energy equation was seen to improve the accuracy of an uncoupled casting model, bettering the predicted air gap formation, and eliminating the previously existing time lag for initial formation of the gap.
Acknowledgments

To Daniela; for bringing a slice of inspiration and beauty into my universe.

I would like to thank my supervisor S. A. Argyropoulos for giving me the opportunity to carry out this work and for his guidance every step of the way. I would also like to thank all the graduate students (you know who you are) that helped me achieve my goals.
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**Nomenclature**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>air gap width in air gap correlations, mm</td>
</tr>
<tr>
<td>b</td>
<td>constant in the air gap correlations, W·m⁻²K·mm⁻²</td>
</tr>
<tr>
<td>B</td>
<td>body force term</td>
</tr>
<tr>
<td>C</td>
<td>constant in the air gap correlations, W·m⁻²K⁻¹</td>
</tr>
<tr>
<td>Cₚ</td>
<td>specific heat, J·kg⁻¹K⁻¹</td>
</tr>
<tr>
<td>CTE</td>
<td>coefficient of linear thermal expansion, K⁻¹</td>
</tr>
<tr>
<td>d</td>
<td>temperature constant in air gap correlations, W·m⁻²K⁻²</td>
</tr>
<tr>
<td>D</td>
<td>inner diameter of mold, m</td>
</tr>
<tr>
<td>D</td>
<td>stiffness matrix</td>
</tr>
<tr>
<td>e</td>
<td>temperature constant in air gap correlations, W·m⁻²K⁻²</td>
</tr>
<tr>
<td>e</td>
<td>strain</td>
</tr>
<tr>
<td>E</td>
<td>Young’s Modulus, N·m⁻²</td>
</tr>
<tr>
<td>f</td>
<td>Expansion rod error, m</td>
</tr>
<tr>
<td>f</td>
<td>fraction</td>
</tr>
<tr>
<td>F</td>
<td>correction factor</td>
</tr>
<tr>
<td>g</td>
<td>gravity, 9.81 m²s⁻¹</td>
</tr>
<tr>
<td>G</td>
<td>shear modulus, N·m⁻²</td>
</tr>
<tr>
<td>h</td>
<td>heat transfer coefficient, W·m⁻²K⁻¹</td>
</tr>
<tr>
<td>H</td>
<td>enthalpy, J·kg⁻¹</td>
</tr>
<tr>
<td>htc (HTC)</td>
<td>heat transfer coefficient, W·m⁻²K⁻¹</td>
</tr>
<tr>
<td>k</td>
<td>conductivity, W·m⁻¹K⁻¹</td>
</tr>
<tr>
<td>k</td>
<td>or conductivity related parameter in the air gap correlations, W·m⁻¹m²K·mm⁻¹</td>
</tr>
<tr>
<td>k</td>
<td>or Boltzman Constant, J·K⁻¹</td>
</tr>
<tr>
<td>K</td>
<td>consistency of the metal</td>
</tr>
<tr>
<td>L</td>
<td>latent heat, J·kg⁻¹</td>
</tr>
<tr>
<td>m</td>
<td>or non-linearity error, m</td>
</tr>
<tr>
<td>m</td>
<td>mass, kg</td>
</tr>
</tbody>
</table>
or a material constant (for the thermo-mechanical equations)
or exponent for dimensionless metal diffusivity term

M

any variable of interest

n

material constant (for the thermomechanical equations)
or exponent for dimensionless mold diffusivity term

p

exponent for dimensionless roughness term

P

pressure, Nm⁻²

q

heat flow, W

q''

heat flux, Wm⁻²

Q

total heat flow, W (for the heat transfer equations)

activation energy, Jg/mol⁻¹

r

r coordinate

or resistivity related parameter in the air gap correlations, W⁻¹ m² K⁻¹

R

or body force term in the r-direction (for the thermomechanical equations)
or thermal resistance, W·m² K⁻¹ (for the heat transfer equations)
or metal-mold roughness parameter (for air gap calculations)
or universal gas constant, Jg/mol⁻¹ K⁻¹

or maximum radius, m

or A/D resolution error, m

s

microstructural state

S

source term

or stability error, m

t

time, seconds

T

temperature, K

TP

thermo-physical properties

u

velocity vector, ms⁻¹

u

displacement in x-direction, m (for the thermomechanical equations)

v

velocity in the energy/momentum equations, ms⁻¹

or displacement in y-direction, m (for the thermomechanical equations)

V

viscous terms

w

displacement in z-direction, m (for the thermomechanical equations)
or width, m (for the heat transfer equations)
x
x coordinate
X
body force term in the x-direction (for the thermomechanical equations)
y
y coordinate
Y
body force term in the Y-direction
z
z coordinate
Z
body force term in the z-direction

GREEK SYMBOLS

\( \alpha \)  
coefficient of linear thermal expansion, K\(^{-1}\)  
or thermal diffusivity, m\(^2s^{-1}\)

\( \beta \)  
density differential term equal to \( \sqrt{\frac{\rho_i - \rho_f}{\rho_i}} \)

\( \delta \)  
magnitude of contraction, m

\( \varepsilon \)  
strain (for the thermomechanical equations)  
or emissivity (for the heat transfer equations)

\( \phi \)  
any generic variable

\( \lambda \)  
thermomechanical parameter defined in equation 2.28, Nm\(^{-2}\)

\( \mu \)  
thermomechanical parameter defined in equation 2.28, Nm\(^{-2}\)  
or viscosity in the momentum equations, Nm\(^{-2}s\)

\( \rho \)  
density, kgm\(^{-3}\)

\( \sigma \)  
stress, Nm\(^{-2}\) (for the thermomechanical equations)  
or Stefan Boltzmann constant, 5.67051 x 10\(^{-8}\) Wm\(^{-2}K^{-4}\) (for heat transfer equations)

\( \theta \)  
\( \theta \) coordinate

\( \theta \)  
body force term in the \( \theta \)-direction

\( \nu \)  
Poisson's Ratio

\( \Gamma \)  
any generic diffusion coefficient
### SUBSCRIPTS

- **a**: axial-direction
- **avg**: average
- **ca**: conduction through air
- **cond**: conduction
- **conv**: convection
- **cv**: control volume
- **d**: delayed
- **e**: elastic
- **eff**: effective
- **exp**: experimental
- **f**: fusion
- **fin**: final
- **harm**: harmonic
- **i**: $i^{th}$ direction, coordinate
- **incr**: incremental
- **init**: initial
- **inst**: instantaneous
- **int**: interface
- **j**: $j^{th}$ direction, coordinate
- **m**: melting, liquidus
  - or outer edge of the mold (for the thermomechanical equations)
- **n**: net
- **o**: initial
- **pc**: phase change
- **s**: solid, solidus
- **sur**: verticle surface area of cylinder wall, $m^2$
- **r**: r-direction
- **R**: recovered
- **rad**: radiation
ref reference point
T thermal
T1-T6 identifiers for thermal resistance terms
v viscous
vm Von Mises' stress
vp visco-plastic
x x-direction
y y-direction
z z-direction
\( \phi \) any generic variable
\( \theta \) \( \theta \)-direction
v viscous

**SUPERSCRIPrTS**

P value at the present time
P+1 value at a future time
P-1 value at a past time
" flux
* dimensionless
Introduction

The motivation and purpose behind the work is briefly examined, and a brief description of the contents of each chapter is presented.

The proliferation of mathematical models which predict the solidification behavior of castings has been immense during the 1990's, as industry continues to discover the benefits associated with numerical simulation. The most prominent of these benefits include an overall decrease in developmental costs, time savings and an overall better understanding of the metals casting process. Despite this apparent success, much effort has been spent custom tailoring many modeling packages to a particular casting set up. Often, a package that has been highly successful at simulating a particular casting operation will fail miserably with a new casting arrangement. This presents a unique paradox. Why would the performance of a mathematical model, solving the same governing equations using the same numerical solver (both of which have been thoroughly tested over decades) fail to properly function with a different metal-mold combination? Furthermore, why have most models performed poorly in the prediction of cooling rate related problems, such as hot tearing and final casting microstructure? This work will address these apparent inconsistencies and demonstrate that much of the problem lies not in the model's numerical calculation scheme, but in the boundary conditions input to the model at the interface between metal and mold.

1.1 Motivation Behind this Work

A moderate change in the boundary conditions imposed at the metal-mold interface in many casting simulations can severely affect the validity of the resulting numerical predictions. When one speaks of temperature boundary conditions defined by heat transfer coefficients, this is true
for a number of reasons. Firstly, temperature boundary conditions during most commercial casting processes are inherently transient. Heat transfer coefficients are initially high and tend to drop off at lower temperatures. Secondly, not one, but several mechanisms of heat transfer occur at the metal-mold interface during solidification and cooling, some of which may, or may not be present at any given time. In addition, the specification of a temperature boundary condition is highly dependent on the casting and mold configuration. For instance, certain metal-mold interfaces will remain in contact, while others will develop extensive air gaps depending on their orientation with respect to gravity. Finally, heat transfer coefficients are very sensitive to both mold and metal materials and the surface characteristics of each. A heat transfer coefficient, which has given good results for a given alloy, may become completely inadequate for a different alloy with a different mold. If one wishes to minimize these errors, the next step towards unification of the complex phenomena associated with modeling casting processes is the coupling of boundary conditions among all related governing equations in a given system. The proper definition of temperature boundary conditions hinges on determining the effect on boundary conditions of certain process variables dictated by coupled governing phenomena.

1.2 Purpose of the Study
The main goal of the work at the outset was to improve the performance of the general casting simulation model. Along the way many other goals were identified and pursued as worthwhile byproducts of the study. A listing of these goals appears below.

- To develop an experimental technique to characterize the formation of the air gap at the metal-mold interface during casting
- To develop an experimental technique to determine the heat transfer coefficient at the same metal-mold interface
- To take a systematic approach (not limited to a specific industrial process) to quantify the heat transfer coefficient-air gap/thermo-physical property/surface roughness relationship across a varying range of metal-mold systems
- To correlate the heat transfer coefficient-air gap relationship using a semi-empirical for all systems, including data available in the literature
- To correlate the heat transfer coefficient-air gap/thermo-physical property/surface roughness relationship in a general non-dimensional form for all data generated in this study
CHAPTER 1: INTRODUCTION

- To develop a mathematical model which will predict the growth of the air gap and use the above mentioned correlation to determine the appropriate temperature boundary conditions on a real time basis
- To apply the model to improve the accuracy of aluminum alloy casting simulations, especially with respect to predictions related to air gap formation (and hence cooling rates)
- To quantify the error in heat transfer coefficient and air gap measurements
- To use the model to predict the air gap formation in a sand casting where experimental methods prove difficult

Some of these goals have been partially explored in other systems by previous research, while others are completely unique to this work.

1.3 Project Overview

A multi-faceted study of this type involves a large scientific knowledge base. Many theoretical concepts were explored in detail before the individual components of the work could come together. For the sake of readability, general theory will be discussed comprehensively in the next chapter, and any further background information needed to understand the contents of each subsequent section will be given on a 'just in time' basis at the beginning of the appropriate chapter when necessary. The areas of expertise involved in this work include:

- Mechanisms of Heat Transfer (conduction, radiation, convection)
- Mechanical Behavior of Metals (low and high temperature behavior)
- Numerical Modeling of Heat Transfer/Fluid Flow/Thermo-mechanical Displacement
- Rheological Behavior of the Mushy Zone in Metals (semi solid processing, thixotropic behavior)
- Statistical Interpretation and Correlation Techniques
- LVDT & Thermocouple Data Acquisition Systems

Many of these areas are foreign territory to the metallurgist and required multi-disciplinary preparation from a variety of engineering fields. A very broad overview of this study appears in Figure 1.1. The main thrust of the work is shown in this six step graphical schematic depicting the transfer of experimental information to a numerical strategy resulting in an improved model,
CHAPTER 1: INTRODUCTION

Figure 1.1: A General Overview of the Project

which shows better agreement with reality. Having outlined many theoretical issues in Chapter 2, Chapter 3 will focus on steps 1 and 2 with the development of the experimental setup, results from the experimental trials, and a description of the methods used to minimize potential errors. In Step 3 a heat transfer correlation is proposed and statistical analysis is used to isolate important variables. This development is outlined in Chapter 4. The final three steps are contained in Chapter 5, which summarizes the formulation of the mathematical model, and the subsequent incorporation of the heat transfer correlation into the numerical scheme. This chapter also contains a general analysis of the results of the work including important applications of the new model. A summary of the important findings of this study appears in Chapter 6, which contains the conclusions of the work.
Background Theory

The basic experimental and numerical theory underlying the work is explained, and the current literature is reviewed.

Current numerical models often claim to solve for all of the major solidification phenomena present during casting. This would include heat transfer, phase change, fluid flow, thermal contraction and shrinkage. Many of these phenomena are coupled (that is the solution of one equation will affect the solution of one or more other equations) and are present only in certain material phases as outlined below in Figure 2.1.

![Diagram of coupled phenomena in metals casting]

Figure 2.1: Coupled Phenomena in Metals Casting
With the recent advance in the modeling capabilities of numerical solidification algorithms [1], it seemed that all that was considered to improve the simulation accuracy of metals being cast was the inclusion of an additional complex phenomenon or the formulation of an additional mechanism into the calculation scheme. While model development and implementation had been receiving most of the attention, a related field, the specification of general boundary conditions, had been largely neglected. As models continue to become more complex, their dependency on accurate boundary conditions intensifies. Unfortunately, research in this area has not been sufficient (this oversight has been documented in earlier works of the author [2][3]). With respect to heat transfer coefficients, current industry practice is either to assign numbers based on past experience with the mold and metal materials (i.e., pick a value until the results look good, then keep that value for future trials), or to use in-house measurements for a particular casting [4]. Both practices are strictly short-term compromises, which do not address the fundamental relationships which exist at the metal-mold interface. In addition, values produced by these solutions cannot be generalized for other processes, and tests must be conducted over and over for each new system. As a consequence, these techniques will not provide the flexibility required by the modeler in the future.

Reality dictates that a host of factors play critical roles in determining model accuracy, and most of today's models are constrained by these additional factors. Can one categorize the set of all factors which influence a model's performance? Generally speaking, one can. The parameters which affect the ability of a mathematical model to simulate a process properly can be related to one of the following three broad categories:

![Figure 2.2: Parameters Governing the Performance of a Casting Model](image)

It is assumed that most mathematical modelers have a good grasp of the first parameter (i) for a particular phenomenon of interest such as heat flow, since mathematical descriptions of
numerous casting phenomena, as in Figure 2.1, have existed for many decades. Converting the mathematics into numerical algorithms, via finite difference or finite element analysis is also a well-established and historically well validated field. Parameter (ii) is the responsibility of the scientific community in general, and as our database continues to expand, the range of materials that can be modeled also grows. In any case, a thorough experimental study can theoretically rectify any thermo-physical property problem. This leaves parameter (iii) as the area where most difficulties can occur between model and reality as illustrated in Figure 2.3.

- **Mathematical Formulation** ✗
  The governing equations which describe the phenomena are mostly well documented and relatively easy to solve numerically

- **Thermophysical Property Specification** ✗
  Though initially a major concern, the development of materials databases will continue to curb this problem

- **Specification of Boundary Conditions** ✓
  One of the most problematic boundary conditions is the heat transfer coefficient and how it varies with time during casting

**Figure 2.3: The Relative Importance of Boundary Condition Specification**

If one ignores the contribution of parameter (ii), as it represents a gradually improving trend, and examine the changes which have lead to the improvement of model performance shown in Figure 2.4, one notes that boundary conditions represent the area where most improvement can be made. The reasons for this inadequacy in the modeling community perhaps stems from an inability on the part of the modeler to study the process himself on an experimental basis, relying solely on the 'experimentalist' for validation. Hence, any lack of communication between the foundryman and the modeler will reflect itself immediately in a discrepancy between process and model.
It is interesting to note that the main difference between a real process and the model that emulates it is that the process cannot isolate itself from the effect of variations in its environment the way a model can, via convenient assumptions. Thus, the likelihood of encountering errors due to boundary conditions is high in comparison with errors in formulation, coding and thermophysical property specification. With modern casting simulation, the need for a method of assigning accurate boundary conditions will become increasingly critical. The most precise model in the world will not be an accurate predictor of process behavior if the numerical input boundary conditions associated with the process are inconsistent with reality.

Accurate heat transfer coefficients are historically difficult to obtain experimentally for all points on the metal-mold interface especially when the influence of thermal contraction is acknowledged. The main focus of this study is an attempt to remedy some of the pitfalls associated with the specification of heat transfer boundary conditions at the outer boundary of the metal. The ultimate goal is to allow the modeler to estimate the effect of changes in the heat
loss at the metal-mold interface, and ultimately to allow the time dependent heat transfer coefficient for a particular metal-mold system to be assessed via a numerical correlation, without resorting to a specific experiment.

To achieve this goal, the processes that take place at the metal-mold interface need to be examined. More specifically, the transient mechanisms of heat transfer at the interface and the formation of the air gap between metal and mold must be understood. Firstly, let’s consider the formation of the air gap.

2.1 Air Gap Formation at the Metal-Mold Interface

Qualitative observations of the formation of an air gap during solidification and cooling of metals have been made since the dawn of casting, but not until the second half of this century have any serious attempts at experimentally detecting the magnitude of the air gap been attempted. Savage [5] was among the first to use an inflection in the cooling curve of the mold near the interface to estimate the instant at which the gap first formed. Another technique, based on the variation of capacitance between a sensor placed on the mold wall and the solidifying casting, was developed by Majumdar, Raychaudhuri and Dasgupta [6]. This technique not only determined the beginning of the gap formation, but was also able to track the change in air gap size as a function of time. Winter et al. [7] used a Vycor probe (a linear transducer) to record both phase change and solid-state shrinkage in aluminum. Despite the success of these early techniques, modern researchers have apparently reached a consensus regarding the best apparatus for air gap monitoring: the Linear Variable Differential Transformer (LVDT).

The use of an LVDT to track the positions of the mold and metal independently, was adopted by researchers as early as the last decade, and has become the most popular technique over the last fifteen years. By the mid 1980s, Isaac, Reddy and Sharma [8] perfected the technique and were able to obtain curves tracking the coordinates of the cast’s outer surface and the interior wall of the mold as a function of time. Afterwards, measurements conducted by Majumdar [6] and Nishida [9] with a variety of metal-mold systems confirmed the potential of the technique. With a complete picture of how the air gap forms, researchers began directing their attention to related
phenomena. Mackenzie and Donald [10] had found a variation in gap formation times and temperatures at different elevations in a casting and most researchers including Lewis and Savage [11] had reached the consensus that the formation of the air gap caused a decrease in the heat loss to the mold wall. Work in this area is still being conducted [12-14].

The preceding pioneering work gave researchers an experimental tool to monitor air gap growth. More recently, however, a second wave of research has been led into describing how the air gap forms mathematically and eventually how its growth with time could be predicted. This vital link would be needed to ultimately include air gap formation data into casting modeling algorithms. The first models originated from the concept of a purely elastic media and subsequent models have expanded on this theme. Thus, it is worthwhile to formulate the general theory of elastic thermal contraction explicitly.

### 2.2 ELASTIC THERMAL CONTRACTION THEORY

A general trend, observed for a long time in nature, is that a substance will ordinarily contract when its temperature drops and expand when its temperature rises. Theoretically, this change can be explained by basic particle theory if one recalls that at higher temperatures, particles have a higher energy and hence vibrate more vigorously. This increase in particle vibration necessitates that each particle will occupy a greater volume of space, and the resulting bulk material will consequently also increase in volume. The extent to which a material expands is directly proportional to its temperature change, and the constant of proportionality, for most materials, remains constant throughout a significant temperature range. This constant of proportionality is known as the coefficient of linear thermal expansion and it is defined as the change in length a rod of unit length undergoes when its temperature is raised one degree Celsius.

Now, how is thermal expansion and contraction related to stress? If the material under consideration is heated uniformly and allowed to expand or contract freely, then no stress will be generated in the body. However, if the material is not heated uniformly, or if the material is constrained in certain directions, then a set of displacements, or system of strains, will be generated at each point within the body, each possessing a unique value. This system of strains is
accompanied by a corresponding system of self-equilibrating stresses known as thermal stresses. In the next section, the relationships between stress and strain are examined.

2.2.1 STRAIN-DISPLACEMENT RELATIONSHIPS
Before the stress-strain relations are defined, it will be useful to express the components of strain in terms of displacements. Local strain is basically defined as a rate of change in the displacement or position of a point within a continuous body. In all future derivations, it is assumed that the displacements are small and do not affect the body's geometry or density. The strains defined in rectangular components are:

\[ e_{xx} = \frac{\partial u}{\partial x}, \quad e_{yy} = \frac{\partial v}{\partial y}, \quad e_{zz} = \frac{\partial w}{\partial z}, \quad e_{xy} = \frac{1}{2} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right), \quad e_{yz} = \frac{1}{2} \left( \frac{\partial v}{\partial z} + \frac{\partial w}{\partial y} \right), \quad e_{xz} = \frac{1}{2} \left( \frac{\partial w}{\partial x} + \frac{\partial u}{\partial z} \right) \quad (2.1) \]

where \( u, v, \) and \( w \) represent displacements in the \( x, y, \) and \( z \) directions respectively. In cylindrical coordinates, the equations are slightly different.

\[ e_{rr} = \frac{\partial u}{\partial r}, \quad e_{\theta \theta} = \frac{1}{r} \frac{\partial u}{\partial \theta} + \frac{1}{r} \frac{\partial v}{\partial \theta} + \frac{1}{r} \frac{\partial w}{\partial \theta}, \quad e_{zz} = \frac{\partial w}{\partial z}, \quad e_{r\theta} = \frac{1}{2} \left( \frac{\partial u}{\partial \theta} + \frac{\partial v}{\partial r} \right), \quad e_{z\theta} = \frac{1}{2} \left( \frac{\partial w}{\partial \theta} + \frac{1}{r} \frac{\partial w}{\partial r} \right) \quad (2.2) \]

Here \( u, v, \) and \( w \) represent displacement in the \( r, \theta, \) and \( z \) directions respectively. When dealing with stress in castings, the preceding relationships allow for better 'air gap formation' visualization during the cooling stage, as the exact position of every point in the casting can be monitored as a function of time. Next, the relationships between stress and strain need to be formulated.

2.2.2 STRESS-STRAIN RELATIONSHIPS
Purely elastic materials exhibit a linear dependence between stress and strain. Typically, if one considers axial loading, then the two are easily related via Young's Modulus \( (E) \):
However, in three-dimensional media, the effect of orthogonal loading must be accounted for via a constant, $v$, known as Poisson's Ratio. The net contribution to the axial strain by an orthogonal load is

$$e_x = \frac{\sigma}{E}$$

(2.5)

Finally, the effect of temperature on strain, as discussed earlier, can be expressed as $\alpha\Delta T$. The summation of each of these terms leads to the following set of stress-strain equations in rectangular coordinates:

$$e_{xx} = \frac{1}{E} [\sigma_{xx} - v (\sigma_{yy} + \sigma_{zz})] + \alpha \Delta T$$

(2.7)

$$e_{yy} = \frac{1}{E} [\sigma_{yy} - v (\sigma_{xx} + \sigma_{zz})] + \alpha \Delta T$$

(2.8)

$$e_{zz} = \frac{1}{E} [\sigma_{zz} - v (\sigma_{xx} + \sigma_{yy})] + \alpha \Delta T$$

(2.9)

$$e_{xy} = \frac{1}{2G} \sigma_{xy}, \quad e_{yz} = \frac{1}{2G} \sigma_{yz}, \quad e_{zx} = \frac{1}{2G} \sigma_{zx}$$

(2.10)

The shear modulus, $G$, plays a similar role in shear loading that Young's modulus does in axial loading. The two are related by the formula:

$$G = \frac{E}{2(1+v)}$$

(2.11)

In cylindrical coordinates, an equivalent set of equations are obtained by substituting the variables $r$ and $\theta$ for $x$ and $y$, respectively, in Equations (2.7)-(2.10). Thus,

$$e_{rr} = \frac{1}{E} [\sigma_{rr} - v (\sigma_{\theta\theta} + \sigma_{zz})] + \alpha \Delta T$$

(2.12)
\[ e_{\theta\theta} = \frac{1}{E} \left[ \sigma_{\theta\theta} - \nu (\sigma_{zz} + \sigma_{rr}) \right] + \alpha \Delta T \quad (2.13) \]

\[ e_{zz} = \frac{1}{E} \left[ \sigma_{zz} - \nu (\sigma_{rr} + \sigma_{\theta\theta}) \right] + \alpha \Delta T \quad (2.14) \]

\[ e_{r\theta} = \frac{1}{2G} \sigma_{r\theta}, \quad e_{r\theta} = \frac{1}{2G} \sigma_{r\theta}, \quad e_{r\theta} = \frac{1}{2G} \sigma_{r\theta} \quad (2.15) \]

Though the preceding equations give a mathematical description of the thermoelastic continuum in a bulk material, a final set of equations is needed to isolate the problem in terms of displacements.

**2.2.3 EQUILIBRIUM EQUATIONS**

The equations of equilibrium are derived purely based upon mechanical considerations. The complete derivation appears in many continuum mechanics texts [15-20] and the final form of the equations are given below in rectangular and cylindrical coordinates.

**RECTANGULAR:**

\[ \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xy}}{\partial y} + \frac{\partial \sigma_{xz}}{\partial z} + X = 0 \quad (2.16) \]

\[ \frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} + \frac{\partial \sigma_{yz}}{\partial z} + Y = 0 \quad (2.17) \]

\[ \frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{yz}}{\partial y} + \frac{\partial \sigma_{zz}}{\partial z} + Z = 0 \quad (2.18) \]

**CYLINDRICAL**

\[ \frac{\partial \sigma_{rr}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{r\theta}}{\partial \theta} + \frac{\partial \sigma_{r\theta}}{\partial z} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} + R = 0 \quad (2.19) \]

\[ \frac{\partial \sigma_{r\theta}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{r\theta}}{\partial \theta} + \frac{\partial \sigma_{r\theta}}{\partial z} + \frac{\sigma_{r\theta}}{r} + Z = 0 \quad (2.20) \]

\[ \frac{\partial \sigma_{r\theta}}{\partial r} + \frac{1}{r} \frac{\partial \sigma_{r\theta}}{\partial \theta} + \frac{\partial \sigma_{r\theta}}{\partial z} + \frac{2\sigma_{r\theta}}{r} + \theta = 0 \quad (2.21) \]
The body force terms \( X, Y, Z, R \) and \( \theta \) can usually be neglected. With the previous set of equations the problem of thermoelasticity is fully defined, however, in order to obtain a meaningful solution, all 6 strain-displacement relations, 6 stress-strain relations, and 3 equilibrium equations must be solved for 15 variables (6 stress components, 6 strain components and 3 displacement components). This presents a difficult problem which, for most situations, must be solved numerically. For the purposes of this work, the primary consideration in developing the proposed numerical model is the ability to predict the position of the casting as a function of time. To achieve this objective, the set of 15 equations presented above can be reformulated in terms of displacement.

2.2.4 DISPLACEMENT FORMULATION OF THERMOELASTIC EQUATIONS
By substituting the stress-strain relations (Equations 2.7-2.9 and 2.12-2.14) into the equilibrium equations (Equations 2.16-2.18 and 2.19-2.21), and substituting the strain-displacement relations (Equations 2.1-2.2 and 2.3-2.4) into the resulting system of equations, the displacement variables \( u, v, \) and \( w \) can be isolated as follows:

**RECTANGULAR**

\[
(\lambda + \mu) \frac{\partial e}{\partial x} + \mu \nabla^2 u - (3\lambda + 2\mu)\alpha \frac{\partial \Delta T}{\partial x} + X = 0
\]

(2.22)

\[
(\lambda + \mu) \frac{\partial e}{\partial y} + \mu \nabla^2 v - (3\lambda + 2\mu)\alpha \frac{\partial \Delta T}{\partial y} + Y = 0
\]

(2.23)

\[
(\lambda + \mu) \frac{\partial e}{\partial z} + \mu \nabla^2 w - (3\lambda + 2\mu)\alpha \frac{\partial \Delta T}{\partial z} + Z = 0
\]

(2.24)

**CYLINDRICAL**

\[
(\lambda + 2\mu) \frac{\partial e}{\partial r} - 2\mu \left( \frac{1}{r} \frac{\partial w_r}{\partial \theta} - \frac{\partial w_{\theta}}{\partial z} \right) - (3\lambda + 2\mu)\alpha \frac{\partial \Delta T}{\partial r} + R = 0
\]

(2.25)

\[
(\lambda + 2\mu) \frac{1}{r} \frac{\partial e}{\partial \theta} - 2\mu \left( \frac{\partial w_r}{\partial z} - \frac{\partial w_z}{\partial r} \right) - (3\lambda + 2\mu)\alpha \frac{\partial \Delta T}{r \partial \theta} + \theta = 0
\]

(2.26)
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\[
(\lambda + 2\mu) \frac{\partial e}{\partial z} - \frac{2\mu}{r} \left( \frac{\partial (rw_\theta)}{\partial r} - \frac{\partial w}{\partial \theta} \right) - (3\lambda + 2\mu)\alpha \frac{\partial \Delta T}{\partial z} + Z = 0 \tag{2.27}
\]

where:

\[
\lambda = \frac{v E}{(1 + \nu)(1 - 2\nu)}, \quad \text{and} \quad \mu = \frac{E}{2(1 + \nu)} = G \tag{2.28}
\]

Also, in the above relations, for rectangular coordinates:

\[
e = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \tag{2.29}
\]

and for cylindrical coordinates:

\[
e = \frac{1}{r} \frac{\partial (ru)}{\partial r} + \frac{1}{r} \frac{\partial v}{\partial \theta} + \frac{\partial w}{\partial z} \tag{2.30a}
\]

\[
w_r = \frac{1}{2} \left( \frac{1}{r} \frac{\partial w}{\partial \theta} - \frac{\partial v}{\partial z} \right), \quad w_\theta = \frac{1}{2} \left( \frac{\partial u}{\partial z} - \frac{\partial w}{\partial r} \right), \quad w_z = \frac{1}{2r} \left( \frac{\partial (rv)}{\partial r} - \frac{\partial u}{\partial \theta} \right) \tag{2.30b}
\]

Equations 2.22-2.30 completely define the elastic state of a continuous medium exposed to a change in temperature for Cartesian and cylindrical coordinate systems.

2.2.5 BOUNDARY CONDITIONS

Three types of boundary conditions can be specified to obtain a unique solution. They are:

1. Displacement Boundary Conditions

2. Stress Boundary Conditions

3. A Combination of Displacement and Stress Boundary Conditions

For boundary condition 1, the values of \(u, v,\) and \(w\) are specified, usually at the outer edges of the medium under consideration. This boundary condition is the simplest designation possible, since the equations are already expressed in terms of displacement variables. However, in practice, this condition is seldom met, as the displacement at the outer edge of the medium is often the
unknown variable of interest. In boundary condition 2, the stress state of the material is specified at a given point. This condition is more difficult to implement than boundary condition 1, since the stress-strain-displacement relations must be used to transform this condition in terms of the variable \( u, v, \) and \( w \). The resulting boundary equation will also be in terms all three variables at once, thus causing additional difficulties in specifying variables separately. Finally, boundary condition 3, a combination of conditions 1 and 2, poses no additional problems than those already mentioned.

In order to solve for these equations, a numerical scheme generally has to be adopted. For simpler one and two-dimensional cases, various substitutions and approximations can often solve the reduced equations. These techniques are discussed elsewhere [21-25]. The derivation adopted for our computational model is given in Chapter 5.

### 2.3 Rheology of Metals

During casting, metals undergo temperature extremes, which can render conventional elastic theory ineffective in accurately describing contraction behavior. The formation of the air gap may reflect not only the elastic differential expansion between metal and mold, but also the contraction of the metal as it changes phases from liquid to solid depending on the orientation of the interface with respect to gravity. Before one can begin to model the phenomena taking place at the metal-mold interface, a good understanding of metal behavior at various temperatures must be established.

#### 2.3.1 Visco-Elastic Behavior

Alloys exist in essentially one of three states during casting: the liquid state, the solid state and the mushy state. Pure metals exist as either solid or liquid. In the simplest sense, the rheological behavior of a solidifying metal can be broadly categorized as in Figure 2.5

In the liquid state, a metal can be typically treated as a Newtonian viscous fluid, with no accumulating stresses and no fixed deformations. A liquid metal will basically ‘take the shape of its container’ and can transmit only hydrostatic pressure. A metal in its completely solid state will often exhibit elastic (and creep) behavior at stresses below yield, and plastic behavior at higher
- **Low Temperature Solid State: Elastic/Plastic Behavior**
  (majority of contraction occurs during this stage)

- **Mushy and High Temperature Solid State: Visco-Elastic/Plastic Behavior**
  (contributes to deformation soon after solidification)

- **Liquid State:**
  *Newtonian Viscous Fluid*
  (no permanent deformation occurs)

---

**Figure 2.5: Basic Metal Rheology**

stresses. The mushy state of a metal has the least well defined properties of the three states, exhibiting a combination of visco-elastic/plastic behavior. Figure 2.6 gives an illustration of how visco-plastic and visco-elastic behavior compare to other more common material responses to load.

Whereas an elastic solid and viscous fluid will show elastic \( \varepsilon_e \) and viscous strain \( \varepsilon_v(t) \), respectively, and a visco-plastic material will show both, a visco-elastic material will have a 'slower' elastic strain and an additional delayed strain \( \varepsilon_d(t) \) component that materializes upon loading and disappears upon unloading during a finite time interval. The extent to which visco-plastic and visco-elastic behavior can influence the formation of the air gap at the metal-mold interface will depend on certain factors, including the metal examined. Much of this theory can be found in more recent texts [26-29].
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Figure 2.6: Idealized Material Behavior

2.3.2 MECHANISMS OF STRAIN IN SOLIDIFYING METALS
The mechanisms responsible for the creation of the air gap at the metal-mold interface of a casting are documented in Figure 2.7. The range in which a particular strain is produced is given at the bottom of the schematic. Note that the solid and mushy zones have been divided into regions that denote a particular rheological behavior. Unfortunately, many of the ‘constants’ used in the governing equations shown vary significantly during cooling are not well defined for most materials as documented by [30]. One group of researchers [31] are attempting to estimate these parameters for many metals using percolation theory [32-33], but the reliability of these numbers remains a concern especially in light of the studies conducted by many authors, most notably Flemmings [34] on the semi-solid processing of metals.

2.3.3 SEMI-SOLID METALS PROCESSING
Recall that most metals can usually be classified as Newtonian viscous fluids above their liquidus point, visco-elastic/plastic solids throughout most of the mushy region and up to a homologous temperature of about 0.4, and elastic/plastic solids down to room temperature [2]. Most of the
difficulty lies in the characterization of metal rheological behavior in the mushy state [35]. Metals in the mushy state are thixotropic, and consequently their mechanical behavior is dependent not only on temperature, strain, and strain rate, but also on their processing history, or more specifically, the current morphology and degree of agglomeration of the solid particles in the mushy region (often termed the microstructural state). Mushy metals can be described as shear thinning and static thickening materials (i.e., the longer shear is applied, the easier the material shears, and the longer the material remains at rest, the more difficult it becomes to shear, up to respective steady state values as in Figure 2.8).

Under rapid continuous cooling conditions, which are found in nearly all commercial casting processes, static thickening behavior is promoted to the extreme, and the viscosity of a mushy metal at a given solid fraction will often be at least an order of magnitude greater than its viscosity when held at a constant solid fraction isothermally. The isothermal behavior of mushy alloys has been well documented of late in studies of semi-solid processing; in fact two conference proceedings have appeared in the last few years totally dedicated to the subject [36-37]. Only the
behavior of continuously cooled mushy alloys will be considered in the model developed herein. For some metals the relationship between stress and shear rate during solidification in the mushy zone has been characterized in a power law form [38], although the true constitutive behavior is still being formalized. Appropriate assumptions will be made in the next section to apply this complex theory in a practical model.

2.4 Thermo-Mechanical Models

The governing equations for mathematically describing the thermo-mechanical behavior of a metal being cast is currently the most controversial, least established and least understood subject area of the casting model. The difficulties and general lack of consensus among researchers in this area was discussed in Section 2.3. As a result, a wide variety of governing equations [58-68] have been proposed to quantify the response of the cast metal while solidifying and during lower temperature cooling. The proposed models can be categorized as belonging to a general class of solutions, as illustrated in Figure 2.9. As evident in this figure, a given thermo-mechanical model falls under one of three broad categories: elastic, elastic/plastic or visco-elastic/plastic; and often
in a sub-category, either comprehensive or simplified. The comprehensive or simplified categories refer to whether the complete set of equations is adopted (comprehensive) or whether a simpler set of governing equations is used (simplified). Often a simplified model will rely on a set of basic assumptions which allow the more comprehensive relationships to be reduced to a 'special case' form thereby reducing the numerical complexity of the problem significantly, while maintaining the essential accuracy of the solution.

In terms of predicting the deformation state of the casting, elastic behavior exerts the most prominent effect, followed by visco-elastic/plastic behavior in the mushy zone, and least importantly, by plastic deformation at temperatures significantly below the solidus temperature. Because of this, the thermo-elastic equations represent the commonality essential to all thermo-mechanical models.
2.4.1 COMPREHENSIVE ELASTIC THERMO-MECHANICAL MODELS

With respect to predicting air gap behavior, a comprehensive elastic model is often an advantageous strategy for predicting overall measurements of thermal contractions. This approach can, however, be very computationally intensive even for the simplest of cases, with the complexity of the solution often not justifying the approximate nature of the solution. The model assumes that the casting and the mold are perfect elastic bodies which deform according to changes in temperature. Despite this crude approximation, a purely elastic model can predict the total thermal contraction of a casting to the satisfaction of the modeler wishing to approximate its effects on the local heat transfer coefficient, depending on thermal gradients and the casting's geometry.

The integration of an elastic model into the numerical scheme of a general casting model is a fairly simple task. For the comprehensive elastic approach, the equations developed in Section 2.2 (Equations 2.22 and 2.23), which were derived in terms of displacement, can be reformulated to illustrate the solution methodology. If, for the sake of simplicity, the coordinate system is a two-dimensional rectangular geometry, and substitutions are made in terms of $u$ and $v$, the resulting expressions become:

\[\frac{\partial}{\partial x} \left( \frac{E}{(1+\nu)} \frac{1-\nu}{1-2\nu} \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{E}{2(1+\nu)} \frac{\partial u}{\partial y} \right) = \]

\[\frac{\partial}{\partial x} \left( \frac{\nu E}{(1+\nu)(1-2\nu)} \frac{\partial v}{\partial x} - \frac{E}{1-2\nu} \alpha \Delta T \right) + \frac{\partial}{\partial y} \left( \frac{E}{2(1+\nu)} \frac{\partial v}{\partial y} \right) \tag{2.31}\]

\[\frac{\partial}{\partial y} \left( \frac{E}{(1+\nu)} \frac{1-\nu}{1-2\nu} \frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial x} \left( \frac{E}{2(1+\nu)} \frac{\partial v}{\partial x} \right) = \]

\[\frac{\partial}{\partial y} \left( \frac{\nu E}{(1+\nu)(1-2\nu)} \frac{\partial u}{\partial y} - \frac{E}{1-2\nu} \alpha \Delta T \right) + \frac{\partial}{\partial x} \left( \frac{E}{2(1+\nu)} \frac{\partial u}{\partial x} \right) \tag{2.32}\]

Next, the equations can be discretized and solved using an iterative scheme. Equation 2.31 is solved for $u$ using an initial value for $v$ of, for example, 0. Equation 2.32 is then solved for $v$ with the latest value of $u$. Then $u$ is solved again, and the process is repeated until convergence is achieved for a particular control volume. The equations are solved for every control volume in
the domain in a similar fashion. The air gap at the mold metal interface is calculated by taking the difference in \( u \) between the metal outer wall and the mold inner wall.

The comprehensive approach was used by Hattel [69-70] to examine elastic stresses generated during die-casting. As mentioned, this technique is completely general, though it is very computationally intensive, and is often considered to be 'overkill' for a simple casting simulation. This is primarily due to the fact that castings generally contract inward during solidification, and hence experience little, if any stresses at the outer walls. Hence, a simpler technique can often be adopted with great success.

### 2.4.2 Simplified Elastic Thermo-Mechanical Models

The simplified, purely elastic approach is case specific to the conditions typical during casting, thus eliminating much of the bulk of unnecessary calculation. It cannot be used as a general method for reasons discussed below.

The simplified approach is an effective technique whose success hinges on the assumption that the solidifying body is allowed to contract freely. In practice, this condition is rarely strictly satisfied, as small internal stress will surely be generated in nearly all cases. However, even if this condition is not rigorously met, the technique will still give acceptable results for most numerical simulations where these stresses will remain relatively small. The basic equation involved in estimating the extent of contraction is given as:

\[
\delta_i = \alpha r_i (T_i - T_{av})
\]

where \( \delta_i \) is the magnitude of contraction in the \( i^{th} \) direction, \( \alpha \) is the coefficient of linear thermal expansion, \( r \) is the distance in the \( i^{th} \) direction between the casting's center of gravity and the interface under consideration, \( T_i \) is the solidus temperature of the cast material, and \( T_{av} \) is the average temperature of the casting.

Equation 2.33 can be expressed in rectangular, as well as cylindrical coordinate systems by substituting \( x, y, r, \) and \( z \) for \( i \).
The only unknown in the above equations is the average temperature of the casting, which must be supplied by an appropriate numerical solidification simulation. The second component necessary for predicting the size of the air gap is the determination of the position of the mold as a function of time. This can be accomplished in a similar manner via the use of the Equation 2.33 for the mold instead of the metal. In this case, the coefficient of thermal expansion becomes that of the mold and $T_i$ becomes the average temperature of the mold at the moment when the casting begins to solidify.

Finally, the thickness of the air gap can be expressed as a difference between the contraction of the casting and mold after any given iteration as

$$A = \delta_{\text{cast}} - \delta_{\text{mold}}$$  \hspace{1cm} (2.38)

The use of the simplified elastic model can be effective for cases where a general picture of the contraction of the casting due to temperature effects is required. It has been adopted by Huang [71] for the casting of horizontal cylinders. For a more representative simulation of casting behavior, non-elastic behavior must be included to account for non-recoverable strain.

### 2.4.3 Elastic/Plastic Thermo-Mechanical Models

Countless elastic/plastic models have been developed in the literature over the last few decades, with a wide variety of plastic behavior constitutive equations being adopted [72-77]. Though a
complete discussion of these models is beyond the scope of this thesis, it suffices to say that the vast majority of these models were developed to account for low to medium temperature effects, and do not concern themselves with materials at or near their melting temperatures. The viscous effects at these high temperatures will effect the overall displacement of the casting to a greater degree than the lower temperature plastic effects which are often non-existent at the low to moderate stresses generated during many casting scenarios.

When one speaks of plastic deformation, it becomes worthwhile to examine which deformation mechanisms are dominant as a function not only of stress, but of temperature as well. In Figure 2.10 a typical Ashby diagram [76] is shown to illustrate the dominant mechanisms of strain for a given stress and temperature value.

![Ashby Diagram]

**Figure 2.10: A Typical Ashby Deformation Diagram**

The diagram illustrates deformation mechanism regimes below the theoretical shear stress of a metal. The uppermost regime, dislocation glide, is the most common form of plastic deformation...
observed at low temperatures, and represents the typical manner in which dislocations move to propagate plasticity. Below this regime and to the right, the phenomenon of dislocation creep dominates. In this regime, the movement of dislocations occurs mostly via higher temperature diffusion to different half planes. The dislocations move by both climb and glide. At even higher temperatures, the main mechanism of deformation is diffusional flow, which is divided into two sub-regions, Coble creep and Nabarro creep. The regime of Coble creep involves the transgranular (along grain boundaries) diffusion of point defects, while the Nabarro regime refers to the intergranular diffusion of point defects through the interior of the crystal itself.

Equivalent Ashby diagrams were constructed by Ganghi [78] for high purity aluminum, commercial purity aluminum, and an aluminum alloy (Hiduminium). During the solidification of castings with simple geometries, such as the cylindrical one-dimensionally cooled casting in this study, the typical path of solidification is shown to pass through the lower stress mechanisms of diffusional and elastic deformation, as in Figure 2.10. This observation has been confirmed by Dour [79], and can be used to simplify the numerical model development considerably. Hence, the use of a low temperature elastic behavior model combined with a high temperature visco-plastic behavior model should satisfactorily predict the deformation behavior of most castings.

**2.4.4 COMPREHENSIVE VISCO-ELASTIC/PLASTIC THERMO-MECHANICAL MODELS**

The comprehensive visco-elastic/plastic thermo-mechanical model is representative of the most ambitious endeavor in modeling casting stresses. In theory, the model involves the solution of the following set of general equations:

\[
\sigma = D(\varepsilon_e) \tag{2.39}
\]

\[
\varepsilon_e = \varepsilon - \varepsilon_T - \varepsilon_v - \varepsilon_{pc} \tag{2.40}
\]

\[
\varepsilon_T = \alpha \Delta T \tag{2.41}
\]

\[
\varepsilon_v = f(\sigma, T, \dot{\varepsilon}, s) \tag{2.42}
\]

\[
\varepsilon_{pc} = \beta \dot{\varepsilon} \tag{2.43}
\]
In Equation 2.39, stress is expressed via the stiffness matrix \( D \) in terms of elastic strain, which is equal to the total strain minus the thermal, viscous and phase-change strain, respectively. The thermal strain is simply the coefficient of thermal expansion times the change in temperature, the phase-change strain is equal to the change in fraction solid times a volumetric contraction constant, and the viscous strain is a function of net stress (stress above a threshold stress), temperature, strain rate and a parameter, \( s \), which represents the particle morphology and degree of agglomeration in the mushy state. Researchers in this area have reached a consensus on the general form of these equations, but where much confusion exists is in the mathematical form of the viscous strain term. A general description of the most current forms of these equations will be briefly outlined.

**POWER LAW FORM**

The power law form of the viscous strain term is essentially an extension of the practical lower temperature power creep law to higher temperatures. The general form of this law is

\[
\sigma = A \cdot \varepsilon \cdot \dot{\varepsilon}^n
\]

where \( A \), \( n \) and \( m \) are the values of material constants. For higher temperatures \( n=0 \) and the equation becomes:

\[
\sigma = A \cdot \dot{\varepsilon}^m
\]

Many values of \( A \) and \( m \) exist for 'traditionally' high temperatures, but for ultra-high temperatures, including the mushy zones of many alloys, these values need to be better established.

Vicente-Hernandez [80] has used this approach to define a viscous strain term given by the modified Norton-Hoff law as:

\[
\dot{\varepsilon}_v = \left( \frac{\sigma_{\text{mt}}}{K} \right)^{\frac{1}{n}}
\]

(2.46)
CHAPTER 2: BACKGROUND THEORY

The K term is defined as the consistency of the metal, m is the strain rate sensitivity coefficient, and the σ_neu term is the Von Mises' stress minus a threshold stress above which visco-plastic flow occurs. The coefficients m and K vary significantly with temperature in the mushy zone soon after solidification, and must be measured precisely at every instant. This technique is quite simple to implement but, as with all the techniques in this section, requires the specification of accurate thermo-physical properties that are difficult to obtain at high temperatures.

POWER LAW AND GAROFALO CREEP

The Garofalo [81] creep equation is a slightly more complex version of the power law equation and has the form:

$$\dot{\varepsilon}_p = A \left[ \sinh \left( \frac{\sigma_{\text{vm}}}{\sigma_o} \right) \right]^n \exp \left( -\frac{Q}{RT} \right)$$

(2.47)

where A is a temperature dependent material constant, σ_{vm} is the Von Mises' stress, σ_o is the threshold stress, n is a material constant, Q is the activation energy, R is the universal gas constant, and T is the temperature. This equation was adopted by Drezet [82-83] and Bellet [84] in combination with the Norton-Hoff law to model the direct chill casting of an aluminum alloy. The Norton-Hoff law was used at extremely high temperatures and Garofalo Creep was phased in as temperatures dropped. Although an improvement over the simple power law expression, this strategy suffers from the same high temperature limitations.

In spite of improved numerical results, all documented studies to date have relied on empirical curve fitting techniques to obtain parameters for a given proposed equation. No analytical models of the mechanisms responsible for strain formation (such as those developed at lower temperatures) have consistently shown good agreement with experimental results. Although uncertainty relating to these concepts will persist for a long time, the general form of the visco-elastic/plastic equations given by Equations 2.39-2.43 will remain a blueprint for future modeling in this area.
2.4.5 SIMPLIFIED VISCO-ELASTIC/PLASTIC THERMO-MECHANICAL MODELS
Because of the complexities associated with a comprehensive visco-elastic/plastic model, a number of researchers have developed models which have reduced the overall computational effort required in producing an approximate visco-elastic/plastic solution. These models make effective assumptions to simplify the comprehensive set of equations, while recognizing the ineffectiveness of a purely elastic approximation.

A simplified visco-elastic/plastic model will attempt to describe the elastic portion of the thermo-mechanical equations in conjunction with a relaxation term to account for viscous behavior at higher temperatures. In effect, the model attempts to account for high temperature mechanical behavior in terms of recrystallization. The net effect is that the stress distribution in the casting is not known with certainty, but the overall deformations are well approximated. This strategy is particularly effective in the case of predicting air gap formation, where the size of the air gap formation is only linked to the ultimate prediction of the outer position of the metal wall.

Purvis [85] developed an effective model of this type based on the main assumption that the material’s relaxation behavior was that of a standard linear solid with relaxation being an adequate substitute for creep at the near liquid temperatures associated with casting. He began with the premise that the casting was free to contract, and the total thermal strain was elastic.

$$\varepsilon_T = \alpha \Delta T$$  \hspace{1cm} (2.48)

If a control volume scheme is used, as shown in Figure 2.11 below, Equation 2.48 can be written in terms of node points as:

$$\varepsilon_i^p = \alpha \left( T_i^{p-1} - T_i^p \right)$$  \hspace{1cm} (2.49)

At this stage the model is a simple-elastic approximation, but a visco-plastic component at high temperatures can be introduced as a relaxation term. The amount of relaxation experienced by each control volume is a function of the time, temperature and stress state of the material. Purvis, for example, introduces a term of the form
Figure 2.11: Control Volumes for the Simplified Visco-Elastic/Plastic Thermo-Mechanical Model

\[ \tau_i^p = \tau_0 e^{\left( \frac{Q}{kT_i^p} \right)} \]  

(2.50)

where \( \tau_{i,j} \) is the relaxation time for each element, \( \tau_0 \) is the limiting value of relaxation time for very high temperatures, \( Q \) is the activation energy, \( k \) is the Boltzman constant, and \( T \) is the temperature of the control volume. Since the amount of strain generated in Equation 2.49 will undergo relaxation, an ‘unrelaxed’ equation for strain can be given by introducing Equation 2.50 into 2.49 as an exponential decay term

\[ \varepsilon_i^p = \alpha \left( T_i^{p-1} - T_i^p \right) e^{-\left( \frac{\Delta t}{\tau_i^p} \right)} \]  

(2.51)

Thus the total amount of elastic stain minus the amount of strain relaxation can be calculated for every control volume. If the contribution of these strains from every control volume is summed up,

\[ \varepsilon_{total}^p = \sum_{i=1}^{N} \alpha \left( T_i^{p-1} - T_i^p \right) e^{-\left( \frac{\Delta t}{\tau_i^p} \right)} \]  

(2.52)
the total strain at the outer wall of our rectangular casting for each time step is obtained. It then becomes a simple matter to add these totals for every time step,

\[ \varepsilon_{\text{total}} = \sum \varepsilon_{\text{total}}^p \]  

leaving us with the total accumulated strain over a given time interval. If one is interested in the stress state of the casting, Equation 2.52 can be substituted into the simple stress-strain relationship to obtain the approximate equation:

\[ \sigma_i = E_{i,\text{eff}} \sum_{i=1}^{N} \alpha (T_i^{P-1} - T_i^p) e^{-\frac{\Delta t}{T_i^p}} \]  

with the effective Young's modulus equal to

\[ E_{i,\text{eff}} = E_a \left[ 1 - \left( \frac{T}{T_m} \right)^2 \right] \]  

where \( E_o \) is Young's Modulus at absolute zero, \( T \) is the instantaneous temperature of the control volume, and \( T_m \) is the melting temperature of the metal.

This approximate solution is quite effective for low stress castings such as those described in Chapter 3, and this strategy will be adopted in formulating a cylindrical model in this work.

### 2.5 Heat Transfer at the Metal-Mold Interface

As air gap formation theory began to mature, subsequent attention was directed to the mechanisms responsible for the drop in heat transfer. It was initially anticipated by Mackenzie and Donald [10] that the governing mechanism for heat transport across the gap was radiation. Ho and Pehlke [39] have shown that conduction and radiation (but not convection since the gap thickness, and hence the Grashof number are minuscule) are both responsible, and today, this is the generally accepted view.
Studies have been done for decades estimating the heat transfer coefficient in a variety of casting systems. Basic measurements were conducted by Kumar [40] with aluminum alloys and by Hao [41] with steel and iron for specific casting situations. The effect of certain variables on the heat loss at the metal-mold interface has also received some attention. El-Mahallawy [42][43] examined the effect of melt superheat and chill material on heat transfer, and Song [44] conducted similar studies by varying gap gas pressures and mechanical loads applied to the castings. Heat transfer coefficients have even been estimated during mold filling by Chiesa [45].

### 2.5.1 THE FOUR STAGES OF INTERFACIAL HEAT TRANSFER

Casting is intrinsically a transient process and the mechanisms of heat transfer at the interface change during the solidification process. This can have significant ramifications for the modeler who fails to take these mechanism changes into account when estimating heat transfer coefficients. The stages are outlined below in Figure 2.12 with equivalent circuit diagrams.

![Diagram of the four stages of interfacial heat transfer](image)

**Figure 2.12: Development of the Air Gap at the Metal-Mold Interface**
CHAPTER 2: BACKGROUND THEORY

Note that when one speaks of an overall heat transfer coefficient, one is referring to a net coefficient incorporating the sum of all heat transfer mechanisms that determine heat flow from the outer surface of the metal to the inner surface of the mold. Stage I occurs immediately after liquid metal is poured into the mold and is shown in Figure 2.12(a). Here the only mechanism of heat flow is conduction from the liquid metal to the mold wall. Note that an interfacial resistance \( R_{T1} \) may exist between the liquid and solid, although this term is usually very small for liquid metal-mold interfaces.

Stage II is characterized by the solidification of a thin shell of metal next to the mold wall as in Figure 2.12(b). The mold and metal show intermittent contact at asperities and the overall heat transfer scenario becomes quite complex. Heat flow from the metal to the mold occurs via three mechanisms, and since this flow will take the path of least opposition, the overall resistance occurs in parallel as shown in the equivalent circuit of Figure 2.12(b).

Explicitly the mechanisms can be described as follows. The first mechanism is conduction through the contacting asperities. Here \( R_{T4} \) is the resistance due to the thickness of the metal asperity (proportional to the conductivity of the metal and inversely proportional to the length of the path of heat flow through the metal asperity). \( R_{T5} \) is the thermal contact resistance at the asperity interface. \( R_{T6} \) is the resistance due to the thickness of the mold asperity (proportional to the conductivity of the mold and inversely proportional to the length of the path of heat flow through the mold asperity). The second mechanism is conduction through the air pockets in between the asperities. Here \( h_a \) is the equivalent heat transfer coefficient representing conduction through the air pocket (proportional to the conductivity of the gas in the gap and inversely proportional to the width of the pocket). \( R_{T2} \) and \( R_{T3} \) are the thermal contact resistances between the metal-air and air-mold, respectively, and can usually be neglected. The final mechanism is radiation, which occurs between the metal and mold wall, with \( h_{rad} \) representing the radiative heat transfer coefficient.

During Stage II, the roughness that exists at the interface complicates the estimation of a heat transfer coefficient by using analytical equations. Some statistical expressions, such as those published by Sridhar [46], Yovanovich [47], and Schneider [48] have been derived for the special
case where two surfaces remain in contact under pressure with each other. In these studies, the heat transfer coefficient between two surfaces is defined as a function of the harmonic mean of the conductivities of the mold and metal, the pressure applied between the metal and the mold, the hardness of the metal and mold and the roughness of the metal-mold interface:

\[ h_{\text{contact}} = f(k_{\text{harm,mean}}, P_{\text{contact}}, \text{hardness}, \text{roughness}_{\text{surface}}) \]  

(2.56)

As soon as the pressure between the surfaces drops to zero (and the slightest gap begins to form), the expressions are no longer suitable. This instant represents the start of Stage III (Figure 2.12(c)).

Stage III occurs as the casting first pulls away from the mold wall forming a undivided air gap between metal and mold. Here, heat flow occurs via conduction through the air gap and radiation between the metal and mold surfaces. Though the metal and mold asperities are no longer in contact with each other, they still dictate the path of heat flow from metal to mold.

Finally, Stage IV is arbitrarily defined as the stage where the gap grows to a size where the asperities (or surface roughness) can be effectively neglected in estimating the flow of heat. This distinction is important in defining the analytical expressions that one is permitted to use to estimate the overall heat transfer coefficient during each stage. For real surfaces, the following analytical expressions are applicable:

**STAGE I**

\[ h = \frac{1}{R_{T1}} \]  

(2.57)

**STAGE II**

\[ h = h_{\text{contact}} \] (as in Equation 2.56)  

(2.58)

**STAGE III**

(no expression available)  

(2.59)

**STAGE IV**

\[ h = h_{\text{cond,gas}} + h_{\text{radiation}} \]  

(2.60)
Here $\sigma$ is the Stefan Boltzmann constant and $\varepsilon$ is the emissivity of the wall surface.

Alternatively, the assumption that the mold and metal are ‘perfectly flat’ can be used to simplify the complexity of the problem. The following analytical expressions define the problem for a perfectly flat interface:

\[ h = \frac{1}{R_{f1}} \tag{2.62} \]

\[ h = h_{contact} \tag{2.63} \]

\[ h = h_{cond, gas} + h_{radiation} \tag{2.64} \]

\[ = \frac{k_{air}}{A} \frac{1}{\varepsilon_{metal} + 1} - 1 \tag{2.65} \]

Note that all stages, including Stage III, can be characterized for flat surfaces. Neglecting the radiative component will not introduce significant error for low temperature systems and small gaps.

The above analytical expression for Stage III and IV (Equation 2.65) will be used to compare theoretical heat transfer coefficient values with the experimental heat transfer coefficient measurements in Chapter 3.

\subsection*{2.5.2 Heat Transfer Models}

The modeling of the temperature distribution in the solidifying cast is critical to obtaining the thermal contraction at the metal-mold interface. Fortunately, modeling in this area is well developed with countless studies over the last few decades [86-93]. The basis behind modeling in this field is the solution of the energy equation, which, in its most general form is
\[
\frac{\partial}{\partial t} (\rho H) + \nabla \cdot \rho \overline{u} H = \nabla \cdot (k \nabla T) + S
\] (2.66)

where \( \rho \) is the density, \( H \) is the enthalpy (with \( dH = C_p dT \)), \( \overline{u} \) is the velocity vector, \( k \) is the thermal conductivity and \( S \) is a source term. The solution of this equation will be outlined in Chapter 5.

### 2.5.3 Phase Change Models

The solution of the energy equation in casting involves accounting for latent heat release during solidification. A variety of techniques have been developed to incorporate the release of latent heat. Some of these strategies are the Apparent Heat Capacity Method, the Effective Heat Capacity Method, source-based methods, enthalpy methods, the Kirchoff Transformation, and the Heat Integration Method. Many of these techniques are discussed in an earlier work of the author [94] [95-102].

### 2.5.4 Fluid Flow Models

Often, where fluid flow effects are important, models have been developed to calculate the velocity distributions in the liquid portions of the metal during the early stages of casting. For these cases the momentum equations (\( n \) equations for \( n \) dimensional flows) and the continuity equation must be solved. The momentum equations are of the form:

\[
\frac{\partial}{\partial t} (\rho u_i) + \nabla \cdot (\rho u_i u_i) = \nabla \cdot (\mu \nabla u_i) - \frac{\partial P}{\partial x_i} + V_i + B_i
\] (2.67)

where \( \rho \) is the density, \( u_i \) is the velocity in the \( i^{th} \) direction, \( P \) is the thermodynamic pressure, \( i \) is the \( i^{th} \) direction, \( V_i \), which can be neglected at subsonic speeds, represents other viscous terms in the \( i^{th} \) direction, and \( B_i \) is a possible body force per unit volume in the \( i^{th} \) direction.

The continuity equation is

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \overline{u}) = 0
\] (2.68)
and is solved in conjunction with the momentum equations. Certain assumption must often be made in solving these equations such as the Boussinesq Approximation (for temperature varying density changes), and a viscosity approximation near the solid-liquid interface for pure metals (to allow for a gradual change in material viscosity from solid to liquid). Fluid flow models have appeared in the work of numerous authors [103-120]. For conventional casting purposes, modeling flow is often necessary only in certain cases. The interested reader is left to the references for more details.

2.5.5 SHRINKAGE MODELS
The final component of casting modeling is the simulation of the shrinkage caused by liquid cooling and changing phase. Although phase-change shrinkage can be accounted for in a thermo-mechanical model, certain situations, such as the formation of pipes in risers, often require more detailed knowledge of the bulk shrinkage in the liquid phase and subsequent feeding movement due to gravity. Various strategies including cell-marker techniques have been developed in the literature [121-125], including the work of the present author [94] to handle large amounts of shrinkage.

2.5.6 MODELS OF THE AIR GAP FORMATION AND EARLY CORRELATIONS
In the late 1980s, with the proliferation of more advanced computational devices, researchers began to model the formation of the air gap. Nishida, Droste and Engler [9] developed one of the first of these models, a purely elastic formulation, to predict the gap formation. The authors also plotted the experimental heat transfer coefficient at the metal-mold interface as a function of time. Other elastic models were developed soon thereafter including the work of Purvis, Kannatey-Asibu and Pehlke [50] and Magnin [51]. By the early 1990s, some of the limitations of simple elastic models were exposed, and more advanced visco-plastic behavior models (Wisniewski and Brody [52]) and visco-elastic/plastic behavior models (Vicente-Hernandez et al. [35]) were developed, culminating with the efforts of Drezet and Rappaz [31][53]. The classic work of Pehlke [39][54] has looked at both heat transfer at the interface and air gap formation.

A few researchers have attempted to correlate heat transfer coefficients with air gap formation. A correlation of this type was attempted by Huang et al. [49] with a purely elastic model, which assumed that the casting was free of internal stress. Verwijs and Weckman [57] had used an
elastic analytical expression in cylindrical coordinates to estimate the size of the air gap and define the appropriate heat transfer coefficient conditions during a D.C. continuous casting process. Gunasegaram [55] and Bellet [56] have independently reported an approximate linear correlation for three time stages during casting. The purpose of this study is to generalize the relationship between air gap formation and the heat transfer coefficient at the metal-mold interface during casting, for a range of metal-mold casting systems.

Chapter References

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Experimental Study and Analysis

The experimental apparatus is specified in detail, including modifications made during the developmental stages. Experimental results, error analysis, and accuracy checks are described.

The experimental component of this study proved to be the most difficult and time-consuming step to perfect. Since no detailed theory on air gap measurement methodology (other than the mention of the devices used) had been established in the literature, the setup needed to obtain a working correlation had to be developed.

3.1 Specification of Experimental Apparatus

An experiment to correlate heat transfer coefficients to air gap size is really two separate experiments conducted at once. The first experiment requires an examination of the system on a ‘thermal’ basis and the second experiment considers the system on a ‘mechanical’ basis. The key device for analyzing the system thermally is the thermocouple, and mechanically it is the linear variable differential transformer. The nature of the thermocouple will be considered first.

3.1.1 THE THERMOCOUPLE

The thermocouple is a device made from connecting (welding) two dissimilar metal leads (usually thin wires) at a point, and using a calibration between the temperature of the tip and the voltage measured across the leads (produced by the Seebeck effect) to estimate the temperature of media surrounding the tip. The operating principles of the thermocouple can be found elsewhere [1].

The diameters of the thermocouple wire and the sheaths used in this study were 0.05mm and 0.254mm, respectively. The thermocouples were contained within hair-like 304 stainless steel
sheaths with AWG 30-0.254mm outer diameters. K-type modules on the data acquisition board specified the numerical calibration relationships.

Although thermocouples have been used extensively in many studies, and their reliability has been generally confirmed, two pertinent issues must be addressed before accuracy concerns related to this work can be satisfied. Firstly, the typical thermocouple suffers from a time lag, i.e., the measured temperature will lag the true temperature at the point of measurement by a value which eventually decreases to zero. This is known as the response time of the thermocouple and is generally measured as the time required to reach 63.2% of the difference between the initial and steady-state temperature after the introduction of an instantaneous temperature change. The response time of the thermocouple is influenced by both the thickness of the wire used (and hence the size of the welded bead), and the media in which the thermocouple is placed. The response time is illustrated for a few sample cases in the Table 3.1.

Table 3.1: Change in Thermocouple Response Time

<table>
<thead>
<tr>
<th>Wire Diameter (mm)</th>
<th>Still Air (38°C-425°C)</th>
<th>Air at 18m/sec (38°C-425°C)</th>
<th>Still Water (38°C-93°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.05 sec</td>
<td>0.004 sec</td>
<td>0.002 sec</td>
<td></td>
</tr>
<tr>
<td>1.0 sec</td>
<td>0.08 sec</td>
<td>0.04 sec</td>
<td></td>
</tr>
<tr>
<td>10.0 sec</td>
<td>0.8 sec</td>
<td>0.40 sec</td>
<td></td>
</tr>
<tr>
<td>40.0 sec</td>
<td>3.2 sec</td>
<td>1.6 sec</td>
<td></td>
</tr>
</tbody>
</table>

source: Omega Engineering Inc.

In the present experiments, the time lag problem does not become an issue, since the thermocouples ultimately used possessed a minute wire diameter (AWG44-0.050mm), liquid metal has a high heat diffusivity (the ability to heat/cool a thermocouple tip quickly), and most importantly, the temperature transients experienced during casting are sufficiently small to insure that no appreciable lag occurs.

A second issue that requires consideration relates to the errors generated by the thermocouple at steady state. These errors include the manufacturer’s limits of error for the thermocouple wire used, cold junction compensation error, the analogue to digital converter resolution (significant
digits), and error generated by the conversion of thermocouple emf to temperature. These are summarized in Figure 3.1.

1. Manufacturer's Limits of Error for Thermocouple Wire

2. Cold Junction Compensation Error

3. A/D Resolution Error

4. Error Related to the Calibration Relationships for Converting EMF to temperature

Figure 3.1: Thermocouple Errors

The overall contribution of the above errors can be estimated by examining the cooling curves at several known temperature calibration points. The data acquisition system was used to measure the melting points of pure water, pure tin, pure lead, and pure aluminum, as shown in Figure 3.2. The melting points of these materials are 273.15K, 505.06K, 600.60K and 933.25K, respectively.

Upon examining each of the cooling curves (Figures 3.3-3.6), the approximate error observed was seen to increase with higher temperatures. The anticipated error as a function of temperature was calculated by fitting a straight line through the plotted errors in Figure 3.7. This error is used in the error analysis study in Section 3.2.

Another source of error related to the use of thermocouples concerns the accurate placement of the thermocouple beads. Thermocouple bead placement error was minimized by specifying that
Figure 3.2: Calibration Curves with the Pure Media: Water, Tin, Lead and Aluminum.

Figure 3.3: Measured Temperature Profile during the Melting of Ice
Figure 3.4: Measured Temperature Profile during the Solidification of Pure Tin

Figure 3.5 Measured Temperature Profile during the Solidification of Pure Lead
Figure 3.6: Measured Temperature Profile during the Solidification of Pure Aluminum

Figure 3.7: Interpolation of Estimated Error from the Temperature Calibration Curves
the mold be manufactured within minimal tolerances (±0.2mm for drilled holes). This tolerance was verified using a Mitutoyo Model CD-6BS digital caliper.

The strategy of adopting minute diameter sheaths minimizes any error associated with thermocouple conduction as suggested in the NANMAC Temperature Handbook [2]. In addition, since the thermocouples are only used to measure relative temperature differences, if a small error is present, it will be factored out when the difference in temperatures is calculated. Figure 3.8 illustrates the temperature measurement at the outer surface of an aluminum casting as it undergoes phase change in a sand mold. This scenario would induce the greatest conduction error, as the thermal conductivity of sand is the furthest from that of the stainless steel sheaths. Nevertheless, no significant conduction error is detected in the temperature measurements, indicating that the use of extremely small thermocouples is adequate for these conditions.

![Figure 3.8: Temperature Profile at the Surface of an Aluminum Casting in a Sand Mold](image-url)
3.1.2 THE LINEAR VARIABLE DIFFERENTIAL TRANSFORMER (LVDT)

As mentioned in Chapter 2, the LVDT has become the preferred device for measuring air gap formation. The operating principles of the typical LVDT were provided by the manufacturer [3]. In short, as the inner core of the LVDT moves, a linear relationship between voltage and position can be used to measure the displacement produced. The two devices ultimately used in our study were identical Schaevitz model 100DC-D LVDTs with nominal linear ranges of 6.0 mm using the manufacturer's recommended CALEX Model 21550 15VDC Power Supply.

The advantages of the LVDT include frictionless measurement, infinite mechanical life, resolution limited only by the precision of the external electronics, and extreme ruggedness. While measuring gap sizes, four main sources of error need to be identified and properly quantified: non-linearity error, stability error, resolution error, and connecting rod expansion error. These are shown in Figure 3.9.

**Figure 3.9: LVDT error**
CHAPTER 3: EXPERIMENTAL STUDY AND ANALYSIS

Non-linearity error for the Schaevitz model 100DC-E LVDT is 0.25% of full range (manufacturer's specifications), which corresponds to an error of ±0.015mm. Stability error relates to the excitation circuitry and was specified as 0.125% of full range (manufacturer's specifications), or ±0.0075mm. In Section 3.4.4, where the LVDT is used to monitor the contraction of tin, the resolution and stability of the LVDT are vividly seen to be well within these limits by almost an order of magnitude. This suggests that the manufacturer's error specifications probably include a high factor of safety. For the LVDT, resolution error is only limited by the electronics used to carry signals to the data acquisition system. In our case for a 16 bit A/D converter this results in an error of about ±0.00003815mm, which is not in the vicinity for being a cause for concern. Connecting rod expansion error, however, is a unique problem, which deserves additional attention. Consider the mold LVDT for example.

In order to measure the position of the mold, the inner core of the LVDT needs to be attached to the surface of the mold wall. A connecting rod has to be used to physically link the LVDT inner core to the mold wall. Ideally, the perfect connecting rod should be completely rigid, since any deformation in the rod would result in a position reading error. In most cases, this does not pose a problem, but unfortunately, during the casting process, the rod is heated significantly, and will expand by an appreciable amount. Two strategies, based on material selection, are available to minimize this error: the use of a quartz connecting rod (which exhibits little thermal expansion) or the use of thin walled high thermal diffusivity tubes.

The quartz connecting rod requires an additional clamping mechanism to fix it to the metal outer surface (since liquid metal will not wet the surface of quartz), and although the quartz itself will reduce the error significantly, the clamping piece will contribute an additional error source.

The use of thin-walled high thermal diffusivity tubes is seen to be more effective. This strategy is based on the theory that although an individual connecting tube will expand, the use of two LVDTs (one measuring the metal outer position and the other measuring the inner mold wall position) will give an accurate relative position of the metal and mold surfaces, and hence an accurate air gap size measurement. This statement is only true if both connecting tubes heat up in the same fashion—hence the need for a thin walled tube with high thermal diffusivity. A sample
calculation of the expected error can be performed via the use of fin theory and is shown in Appendix I for our 1.25mm outer diameter, 1.05mm inner diameter connecting rod. The maximum error expected is slightly less than one one-hundredth of a millimeter. So, despite not knowing the absolute position of either the metal outer wall or the mold inner wall, the resulting difference between the two readings, which is our air gap size, will be accurate.

Since the LVDTs are used to measure relative changes in position, the exact starting position of the probe is not required, and calibration error can be avoided. The LVDT unit is isolated from the mold by about 30 cm of air, which results in no appreciable temperature rise in the unit.

A plot of a typical output of an LVDT (Schaevitz model 5000DC-E) measuring the formation of an air gap in a large casting is shown below in Figure 3.10.

![Figure 3.10: A Typical LVDT Air Gap Measurement Plot](image)

Notice that the mold and metal interfaces move at the same rate after pouring, since the solid mold expands upon heating and the liquid metal takes the shape of the expanding mold. After a short while, the metal solidifies and begins to contract, while the mold continues to expand to a
maximum before beginning to cool again. One additional consideration needs to be addressed at this stage concerning the difference in LVDT behavior with a change in the metal being cast. If the metal cast is a pure metal, the solidifying shell will ‘clasp’ the LVDT connecting rod immediately upon solidification, and the readings will accurately reflect the outer wall position. This effect is illustrated in Figure 3.11.

![Diagram of clasp effect](image)

**Figure 3.11: The LVDT Connecting Rod**

If the metal cast is an alloy with, for example, a large mushy zone, the ability of the softer metal to ‘clasp’ the connecting rod is compromised, until the metal cools to a lower temperature. This phenomenon will cause an additional distortion to appear initially in the air gap formation, probably resulting in a gap size that is underestimated and more erratic during the early stages. Whether this error is significant or is of a scale, which cannot be distinguished from other general errors, such as imperfections in the assumed planar wall, remains to be proven. The error disappears early in the casting process, however, as the casting solidifies first from the outer shell and is soon able to draw the LVTD connecting rod inward. Experimental results plotted in subsequent sections of this study may indicate that, for very early times, a poorer correlation is achieved for alloys than for pure metals.
3.1.3 Calculating Heat Transfer Coefficients from Thermocouple Data

In order to calculate heat transfer coefficients during casting, one of two techniques can be employed. The first technique involves measuring temperatures in the bulk mold and metal at various internal points, and using an inverse technique to estimate the surface temperatures and temperature gradient. This is known classically as the inverse method [5-6]. The energy balance technique, alternatively, attempts to monitor the temperatures at the inner and outer surfaces of the interface and a short distance into the mold to calculate a gradient. By performing an approximate energy balance at the interface, for small $\Delta r$:

\[ q_{\text{conv, int}} = q_{\text{cond, int}} \]  
\[ h_{\text{int}} (T_{\text{metal, int}} - T_{\text{mold, int}}) = k_{\text{mold}} \left( \frac{T_{\text{mold, int}} - T_{\text{mold, (int-\Delta r)}}}{\Delta r} \right) \]  
\[ h_{\text{int}} = \frac{k_{\text{mold}}}{\Delta r} \left( \frac{T_{\text{mold, int}} - T_{\text{mold, (int-\Delta r)}}}{T_{\text{metal, int}} - T_{\text{mold, int}}} \right) \]

In comparison, the inverse technique is very stable, but is computationally more intensive and has a slower response time (since any heat change must penetrate to the first embedded thermocouple to be detected). The heat balance technique can be more erratic at times, yet it is very efficient and has a fast response to changes in heat flux. An illustration of the relative difference between the two techniques is given in Figure 3.12 below.

Ideally, however, one would not want to measure the temperature gradients from the casting side of the interface, especially within small castings, since at lower cooling rates these castings can behave as lumped masses, where any temperature gradients may approach or exceed the error limits of the thermocouples. In addition, the latent heat effects will further distort the generated temperature profiles from thermocouples placed in the casting.
3.2 Quantification of Error Sources

As illustrated in the previous sections, measurements of many of the parameters in this study include certain error. Depending on the metal-mold system considered, the relative magnitude of total error has the potential to vary considerably. In this section, the total error present in our system is quantified. The result of this analysis will allow us to estimate tolerances that can be quoted when applying our correlations.

Error in this study can be generally categorized as either experimental error or residual error. Experimental error consists of inaccuracy caused by the data acquisition system and measurement devices. These errors can be broken down into thermocouple error and LVDT error. From the individual error contributions of both these devices (discussed in Section 3.1), propagation of error analysis can be used to calculate the overall error in the heat transfer coefficient and the air gap position values. Residual error, alternatively, is a function of the curve fitting procedure used to generate the correlations and will be discussed in Section 4.4. Propagation of experimental error will now be examined in detail.
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3.2.1 PROPAGATION OF EXPERIMENTAL ERROR
Sections 3.1.1 and 3.1.2 outlined the error associated with the specific thermocouples and LVDTs employed in the set up. In calculating our heat transfer coefficients and air gap sizes, propagation of error is analyzed in two ways, as maximum error and as probable error.

Maximum propagation of error will occur when every potential uncertain measurement in a system contains an error equal to its maximum possible error, and each of these maximum errors are assumed to be alternatively all positive and all negative to yield the highest overall positive and negative propagated error. Mathematically, maximum error is defined as:

\[ dM = \sum_{i=1}^{n} \frac{\partial M}{\partial x_i} \Delta x_i \quad \text{(for } n \text{ variables)} \]  \hspace{1cm} (3.4)

where \( M \) represents the equation used to calculate the value of interest, \( x_i \) represents the set of variables in the equation, and \( \Delta x_i \) represents the absolute value of the maximum uncertainty associated with each variable. For example, in calculating the heat transfer coefficient via the energy balance given in Equation 3.3, the maximum propagation of error equation would yield:

\[
\frac{dh_{int}}{dk_{mold}} \Delta(k_{mold}) + \frac{dh_{int}}{d\Delta r} \Delta(\Delta r) + \frac{dh_{int}}{dT_{mold,int}} \Delta(T_{mold,int}) \\
+ \frac{dh_{int}}{dT_{mold,(int-\Delta r)}} \Delta(T_{mold,int}) + \frac{dh_{int}}{dT_{metal,int}} \Delta(T_{metal,int}) \]  \hspace{1cm} (3.5)

and by differentiating,

\[
\frac{dh_{int}}{d\Delta r} = \left[ \frac{1}{\Delta r} \left( \frac{T_{mold,int} - T_{mold,(int-\Delta r)}}{T_{metal,int} - T_{mold,int}} \right) \right] \Delta(k_{mold}) + \left[ \frac{k_{mold}}{(\Delta r)^2} \left( \frac{T_{mold,int} - T_{mold,(int-\Delta r)}}{T_{metal,int} - T_{mold,int}} \right) \Delta(\Delta r) \right. \\
+ \left. \frac{k_{mold}}{\Delta r} \left( \frac{1}{T_{metal,int} - T_{mold,int}} \right) - \frac{k_{mold}}{\Delta r} \left( \frac{T_{mold,int} - T_{mold,(int-\Delta r)}}{(T_{metal,int} - T_{mold,int})^2} \right) \right] \Delta(T_{mold,int}) \]
the working form of the maximum propagation of error equation is obtained. Similarly, the maximum and minimum values of the air gap size can be calculated from the worst case LVDT error. The maximum propagation error for the LVDT is:

\[
dP = \frac{dP}{dE} \Delta(E) + \frac{dP}{dL} \Delta(L) + \frac{dP}{dS} \Delta(S) + \frac{dP}{dR} \Delta(R)
\]  

(3.7)

or

\[
dP = \Delta(E) + \Delta(L) + \Delta(S) + \Delta(R)
\]  

(3.8)

where P is the position of the LVDT rod at the wall surface, E is the expansion rod error, L is the non-linearity error, S is the stability error, and R is the A/D resolution error.

In summary, each thermocouple reading is assumed to be reporting a measurement with either its highest positive or negative potential error, and is positioned with a maximum positive or negative placement error, in a mold whose conductivity will have the highest error from the assumed value, such that the resulting heat transfer coefficient calculation yields a maximum or a minimum value. Each LVDT also exhibits its greatest non-linearity, worst stability, and highest connecting rod expansion and A/D converter error. Though not realistic, maximum error serves to define the theoretical upper limit, under which total error can always be maintained. In practice, it is not reasonable that such an error will be realized. Hence, the concept of probable propagation error is introduced.
Probable propagation error is a measure of the most likely propagation error resulting from the use of an equation where variables exhibit uncertainty. The formula for probable propagation error is defined as:

$$dM = \left[ \sum_{i=1}^{n} \left( \frac{\partial M}{\partial x_i} \Delta x_i \right)^2 \right]^{1/2} \quad \text{(for n variables)} \quad (3.9)$$

which differs significantly from Equation 3.4, in that the total error is calculated by the square root of the sum of the squares of each individual variable's error contribution. The result is that this error is more indicative of the expected error in the equation. For the heat transfer coefficient calculations, Equation 3.9 yields:

$$d_{h_{int}} = \left\{ \left[ \frac{d_{h_{int}}}{dk_{mold}} \Delta (k_{mold}) \right]^2 + \left[ \frac{d_{h_{int}}}{d\Delta r} \Delta (\Delta r) \right]^2 + \left[ \frac{d_{h_{int}}}{dT_{mold,int}} \Delta (T_{mold,int}) \right]^2 \right\}^{1/2} \quad (3.10)$$

or

$$d_{h_{int}} = \left\{ \left[ \frac{1}{\Delta r} \left( \frac{T_{mold,int} - T_{mold,(int-\Delta r)}}{T_{metal,int} - T_{mold,int}} \right) \right] \Delta (k_{mold}) \right\}^2$$

$$+ \left\{ \left[ \frac{k_{mold}}{(\Delta r)^2} \left( \frac{T_{mold,int} - T_{mold,(int-\Delta r)}}{T_{metal,int} - T_{mold,int}} \right) \right] \Delta (\Delta r) \right\}^2$$

$$+ \left\{ \left[ \frac{k_{mold}}{\Delta r} \left( \frac{1}{T_{metal,int} - T_{mold,int}} \right) - \frac{k_{mold}}{\Delta r} \left( \frac{T_{mold,int} - T_{mold,(int-\Delta r)}}{(T_{metal,int} - T_{mold,int})^2} \right) \right] \Delta (T_{mold,int}) \right\}^2$$
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For the LVDT position calculations, Equation 3.9 yields:

\[
\frac{dP}{dE} = \left( \frac{dP}{dL} \Delta(E) \right)^2 + \left( \frac{dP}{dS} \Delta(L) \right)^2 + \left( \frac{dP}{dR} \Delta(S) \right)^2 + \left( \frac{dP}{dR} \Delta(R) \right)^2 \right)^{1/2}
\]

(3.11)

or

\[
dP = \left( [\Delta(E)]^2 + [\Delta(L)]^2 + [\Delta(S)]^2 + [\Delta(R)]^2 \right)^{1/2}
\]

(3.12)

Since the limits of error for each variable in the experimental set up are well defined, the use of probable error (Equations 3.11 and 3.13) is a more practical measure of the anticipated error. Probable error will appear in the plots of Chapter 3, and maximum error is given in Appendix III. Figure A3.7 in Appendix III illustrates the maximum scatter apparent in both the heat transfer coefficient and the LVDT measurements, separately, for data from an aluminum-copper system trial. The original data points are shown in dark, while the maximum error is given as a gray area above and below the actual curve (the gray area is actually a set of error bars, but since the data points are so close together, it appears as a shaded region). The scatter in both curves is very low for the aluminum-copper system, in comparison to the absolute magnitude of each measure valued. Note the positive bias in the LVDT error bars. This is due to the fact that thermal contraction error acts only in the positive direction and cannot add to negative error. The equivalent plot of probable error is given in Figure 3.33(a). The observed error in both plots is quite acceptable for the purposes of defining a working relationship between the variables.
Alternatively, the scatter can be shown in a correlation plot of heat transfer coefficient vs. air gap size using both y and x error bars. A combined plot of the maximum error in the aluminum-copper data is given in Figure A3.8 in Appendix III. Again the magnitude of the experimental error is seen to be small in both x and y for this system.

This result, however, is not always the case. For the equivalent plots of the tin-graphite system (Figures A3.5 and A3.6 in Appendix III, and Figure 3.31(a)), the situation changes dramatically. Here the level of relative variance is extremely large, especially for the LVDT air gap size measurement, as the upper and lower maximum errors are the same order of magnitude as the size of the gap itself. The limits for the heat transfer coefficient measurements are small, but overall, the reliability of this data is much more questionable. The situation improves only marginally when examining the probable error plot, Figure 3.31(a). Despite this observation, the data for the tin-graphite system plot did not deviate from the observed trends in the curves of the other metal-mold systems. The high relative error is seen in Figure A3.6 in Appendix III, where the correlation curves for the heat transfer coefficient as a function of air gap size show a pattern which cannot be confirmed with absolute certainty, due to the high error bar spread. It should be remembered, however, that the tin-graphite system is an extreme case where the casting shows very little shrinkage. The error bar plot confirmed the suspected uncertainty with this system, which was discussed in Section 3.4.4.

From complete set of error bar plots given in Appendix III, the following trends emerged:

- Progressing from systems characterized by higher temperature gradients to systems with lower gradients, the heat transfer coefficient error bars became progressively smaller.

- The LVDT error bars were of a constant magnitude. Thus, systems that experienced less thermal contraction exhibited a greater relative error, culminating with the huge variance in the tin-graphite system.

- The heat transfer coefficient error bars were highly dependent on the relative temperature differences measured between the metal surface and in the mold wall. As time increased, these differences dropped and the magnitude of the error bars increased. This increase
explains the upward drift in the heat transfer coefficient curves for the aluminum alloy-copper systems at later times.

- Of all the correlations, only the tin-graphite system exhibited variance that could render the relationship uncertain. The variance in the A356-graphite system was also high, possibly accounting for the unexplained changes in the curve's slope at various points.

### 3.2 General Experimental Procedure and Apparatus

A graphite crucible was packed with solid slabs of metal and placed within a Bradely coreless induction furnace (shown in Figure 3.13).

![Image of the Bradely induction furnace](image)

**Figure 3.13: The Induction Furnace**

The furnace was used to melt the metal and elevate its temperature to 800°C for aluminum and aluminum alloys, and 400°C for pure tin. These superheats were specified relatively high to allow for sufficient time in transferring the liquid metal to the mold for pouring. Thus, the pouring
temperature was assumed to be about 750°C for aluminum and aluminum alloys and about 350°C for tin. When the desired superheat was reached, the power of the induction furnace was turned off to minimize any electrical interference between the furnace and the data acquisition system. The graphite crucible was raised from the furnace using a pair of tongs and placed on the pouring pocket of the special tilt apparatus. The mold was filled immediately within about 3 seconds and any transient mixing subsided within a second or two. The metal was allowed to cool for at least 250 seconds as the thermocouples and LVDTs collected data every 0.5 seconds. The analogue signals from the thermocouples and LVDTs were sent to a μMac-6000 data acquisition system [4], and ultimately to a PC host for permanent storage. The μMac-6000 contains its own dedicated CPU and is programmed via μMac basic. The data acquisition system was capable of 16 bit resolution, more than adequate for our purposes. This preliminary setup is shown in Figure 3.14 for a sand casting.

Figure 3.14: A Preliminary Experimental Setup
While the general casting procedure remained similar, many modifications to the original positioning of the data acquisition devices and to the mold configuration were made. These changes will now be outlined.

### 3.3.1 Preliminary Experimental Trials

This section outlines some of the difficulties encountered during the experimental trials. Though most of these problems have been eventually overcome, this section will be invaluable to the researcher beginning work in this field. The problems are described on a narrative basis with a reference to experimental trials.

### 3.3.2 Initial Experiment

The initial experiment attempting to collect data was set up as in the following schematic:

![Initial Mold Configuration](image)

**Figure 3.15: Initial Mold Configuration**

The first trial was conducted using commercial purity aluminum cast in a graphite crucible at a superheat of approximately 40°C. From experience with most preliminary attempts of this nature, many difficulties were anticipated, and a change in some of the details of the set up was expected. In this respect, the first trial did not disappoint. From a glance of the temperatures recorded by the four thermocouples in Figure 3.16 below, the first problem became apparent.
Figure 3.16: Thermocouple Readings during the Initial Trial

The pouring temperature of the aluminum was quite low, and the metal began to solidify immediately upon contact with the mold. In order to obtain thorough data on the formation of the air gap, the poured metal should reach a quiescent state before solidification begins to occur. In this way the formation of the gap can be observed in its entirety, and the thermocouple readings have a chance to properly stabilize. The heat transfer coefficient calculated on the basis of these thermocouple readings was very erratic and did not reflect the true nature of the cooling. The solution to this problem is quite obvious: increase the superheat of the poured metal.

Another problem became evident when examining the displacement curves of the mold and metal generated by the LVDTs. The plot appears in Figure 3.17 for millimeters vs. seconds. Two LVDTs of differing overall resolutions were used in this study and one can see that the LVDT used to record the position of the mold did not have sufficient resolution to provide a smooth curve. In other words, a more sensitive LVDT was needed. Before this option was exercised, however, some software-based signal filtering was attempted, and the curve below was produced by taking a 6 period running average of the curve in Figure 3.18 to smooth out the response of the coarser LVDT.
This improved the situation considerably, but for the purposes of ultimately correlating this data with a heat transfer coefficient, the curve was still too 'rough'. Increasing the period used in the filtering showed little change, and it was decided that an LVDT identical to that used to record the metal position should be used.

At this point, a further consideration arose: What guarantee existed that the metal would contract towards its axis of symmetry as it cooled? Unless the metal was fixed at its axis, it could
conceivably contract more towards one side of the mold, depending on how it shifted during solidification. To remedy this problem, a small hole was drilled at the bottom of the mold along the axis of symmetry. This allows liquid metal to pour into the hole and act as a holding pin upon solidification. Other symmetry concerns are addressed in Section 3.3.4.

3.3.3 SUBSEQUENT EXPERIMENTS

Armed with the preceding improvements to the set up, the next experiment proved to be considerably more successful. The formation of the air gap is shown in Figure 3.19.

![Figure 3.19: Improved LVDT Readings the Second Trial](image)

The addition of the more precise LVDT improved the stability of the mold position output, and fixing the cast to its axis of symmetry gave very clean results with respect to the formation of the air gap. Thus, the displacement measuring apparatus was performing to our expectations.

However, difficulties still remained with the temperature data acquisition set up. After analysis, the temperatures recorded at the interface proved to be somewhat inaccurate. Unfortunately, when taking sensitive measurements for heat transfer coefficient estimation, slight inaccuracies are often enough to blur true trends. Up to this point, the temperature of the metal at the interface and the temperature of the mold at the interface were recorded by positioning the two interface thermocouples as shown in Figure 3.20.
Figure 3.20: Initial Placement of Interface Thermocouples

Although it looks feasible, this setup has a host of inherent errors. Firstly, the physical size of the thermocouple tip allows metal to come in contact with thermocouple B causing an immediate error in the temperature reading. Secondly, because the thermocouple is placed from within the melt, as the metal solidifies and contracts, it will pull the thermocouple from the mold wall and the thermocouple will no longer read the mold wall temperature. Thirdly, the temperature gradients in the metal are not as high as those in the graphite mold wall, and both the relative resolution error of the thermocouples and the positioning error could be reduced by measuring the gradients from the mold side. A final incentive to remove thermocouple B from within the melt is the reduction of thermal field distortion from the presence of the thermocouple shaft. Although the presence of some thermocouples in the melt is necessary to measure interior metal temperatures, the fewer thermocouples required, the better. Thus, the thermocouples were subsequently inserted from the side as shown in Figure 3.21.

The diameters of the new thermocouple wire and their sheaths were 0.05mm and 0.254mm, respectively. The minute diameters insured that thermal conduction error was kept to a practical minimum. Another change to the configuration was necessitated by a geometrical concern. Because the measurements of the heat transfer coefficient and air gap size need to be indicative of the values normal to the surface of the interface, the system had to be modified such that the top and bottom end effects could be neglected. This was accomplished by two changes: the aspect ratio of the casting was increased to a value of 10 to 1, and insulation was added to the top and
bottom of the cylindrical casting. With these changes, the system behaved one-dimensionally, with all values varying in the radial direction only. Thermally, this would mean no gradients in the z-direction and perfect uniformity about the axis of symmetry. Mechanically, this would imply that the stresses generated in the casting are planar, and all contraction occurs towards the center.

At this point it was assumed that most of the difficulties had been overcome, unfortunately however, this did not prove to be the case. For the sake of brevity, the errors detected and subsequent modifications made will be outlined concisely in an abbreviated format in the next section, and a summary of all important modifications will appear afterwards in Table 3.2. The three most important modifications are highlighted in Figure 3.22.

3.3.4 ADDITIONAL MODIFICATIONS/FINAL EXPERIMENTAL SET UP
Insulating the mold proved to be the cause of a particularly stubborn problem. The bottom of the mold was insulated in the following manner: the mold base was removed leaving a mold, which was essentially now a thick walled cylindrical tube. Ultra low-diffusivity refractory material was fitted to the base of the mold and a reverse pin was drilled into the insulation at the axis of symmetry. The top of the mold was insulated via a similar cap. After running a trial with the newly insulated mold, the temperature profiles improved dramatically, especially for longer times.

Figure 3.21: New Positioning of Thermocouples
The air gap measurement readings, however, became completely irregular. At first, no logical explanation for the failure of the devices could be envisioned, and many trials were conducted using different techniques to bind the insulation to the mold. Finally, the reason behind this anomaly was recognized. The mold and the insulation were made from drastically different materials with drastically different coefficients of thermal expansion. Thus the mold base was expanding and contracting at a different rate than the mold wall, and this difference was enough to completely disrupt the validity of the readings. The solution was to construct the mold with a thin base of the same material as the mold walls (to maintain uniform structural continuity during expansion) and place the insulation immediately below the thin base (to supply a sufficient insulating effect).

Other trials were conducted to determine the optimum placement of the LVDTs. Studies from the work of Vicente-Hernandez [17], Bellet [8] and Gunasegaram [7] indicated that experimental temperature and LVDT readings taken in a cylindrical mold, with a casting bound at the axis of symmetry, did not differ according to the $\theta$ angle (around the axis of the cylinder) for a given radial position. These studies employed multiple LVDT set-ups to confirm the radial symmetry of the cylindrical geometry. Thus, the preferred orientation was selected with both LVDTs on
the same side of the casting one slightly above the other. Three independent trials were conducted in the same metal-mold system in this study to further validate this assumption. In the worst case, symmetry error will not exceed the ratio of the pin diameter to the casting diameter, which translates to 0.75 cm/6 cm or 12.5% error for the sand mold, and 0.5 cm/6 cm or 8.3% error for the graphite and copper molds.

Perfecting the thermocouple setup required even more tests. The mold interior thermocouples were placed in precision drilled holes, with the mold interface thermocouple less than a millimeter from the inner mold wall. The holes drilled to house the thermocouples (and hence the thermocouples themselves) were of minimal diameter so as to cause the least possible disruption to the resulting thermal field in the mold wall. The technique used to properly place the thermocouple measuring the metal outer temperature required adopting a unique trick perfected after several trials. The thermocouple was passed into a hole drilled completely through to the inner wall of the mold cavity, until the thermocouple tip protruded just enough into the mold cavity to allow the liquid metal to weld the tip to the outer wall of the casting. The thermocouple was allowed to slide freely so, as the casting contracts, it pulled the thermocouple with it. Here the proper positioning of this thermocouple could be verified afterwards via an inspection of the cast surface.

A final implemented change enhanced the performance of the remaining mold thermocouples via spring loading. This insured that, as the mold expanded and contracted, intimate contact between the thermocouple and the mold would be maintained. The final experimental set up is given in Figure 3.23. A summary of these relevant modifications is given in the Table 3.2, and can serve as a checklist for future work in this area.

For sand molds, the use of insulation was not practical (since sand is a good insulator itself). Thus, the dimensions of the mold were extended by a factor of two in the z-direction. The mold dimensions for sand are given in Figure 3.24. The dimensions for graphite and copper molds are about half the height of those shown for sand with a 0.5 cm diameter pin hole, but otherwise identical (i.e. inner diameter of 6 cm, outer diameter of 20 cm, height of 30 cm).
Figure 3.23: Final Experimental Setup

The experimental trials were conducted without the use of washes at the mold inner surfaces. No welding occurred, as the aluminum did not readily diffuse into the copper wall during the time it was in its liquid state.

3.3.5 CHECK FOR ONE-DIMENSIONALITY OF THE SYSTEM
As mentioned previously, the requirement of one-dimensional heat flux radially outward is essential for obtaining meaningful results. Eventually with time, despite efforts to change aspect ratios and insulate, end effects will render our results less and less legitimate. Ideally, one has a window of opportunity in which to take temperature measurements, after which the data will begin to show appreciable departure from one-dimensionality. Usually this can be seen when the normally monotonically decreasing value of the heat transfer coefficient starts to increase, but this is not a reliable measure by any means.

To solve this problem and estimate the duration of 'one-dimensional conditions', a numerical solution to the conduction problem in a cylinder considering only the thermal properties and the geometry of the metal-mold system was executed. The results for aluminum cast in a graphite mold are shown below in Figure 3.25 where,
Table 3.2: Precautions for Proper Design of Air Gap/Heat Transfer Coefficient Measurement Experiment

<table>
<thead>
<tr>
<th>PRECAUTIONS</th>
</tr>
</thead>
<tbody>
<tr>
<td>THERMAL</td>
</tr>
<tr>
<td>Since the heat transfer coefficients at the interface must be calculated for one-dimensional heat flow to be meaningful, the system must be cooled unidirectionally perpendicular to the flow of heat. This is achieved by increasing the casting aspect ratio (limited by the need to measure appreciable air gap sizes) and by adding insulation to the top and bottom of the mold.</td>
</tr>
<tr>
<td>The thermocouples should be of minimal outer diameter to reduce their heat capacity, and be spring loaded to maintain intimate contact with the mold during expansions and contractions.</td>
</tr>
<tr>
<td>MECHANICAL</td>
</tr>
<tr>
<td>To obtain a uniform air gap around the casting, its geometric center must remain fixed. This is facilitated by the pin in Figure 3.23. The materials forming the base of the mold should be made of thin sections as to not absorb significant heat from the bottom in the axial direction, and cannot be made of a different material than the rest of the mold (i.e., an insulator) since the contraction of the mold, and hence the air gap formation, will be altered.</td>
</tr>
<tr>
<td>The extension of the LVDT rods should be made of a relatively low thermal expansion material (like quartz) for absolute measurements, or of a thin walled tube (which cools to the mold temperature within a few mm of the interface) for relative measurements.</td>
</tr>
</tbody>
</table>

\[ T^* = \frac{T - T_{\text{ambient}}}{T_{\text{initial}} - T_{\text{ambient}}} \]  

(3.14)

is the dimensionless average temperature of the casting, equal to 100% at initial pouring and equal to 0% at room temperature. Note that at \( T^* = 85\% \) the temperature iso-contours are essentially vertical at the top axis of symmetry (where experimental measurements are taken) indicating heat flow is radially outward, perpendicular to the iso-contours. This pattern continues strongly until \( T^* = 30\% \) which is the last point where our 1D approximation is good. If one continues beyond this point, two-dimensional effects become apparent soon afterwards at \( T^* = 20\% \), with a change in the slope of the temperature iso-contours at the top axis of symmetry. For aluminum/graphite systems this corresponds to about 500 seconds, which is reduced to 250 seconds to be completely safe.
Figure 3.24: Mold Dimensions for Sand Casting

Figure 3.25: Modeled cooling Histories of a Cylindrical Casting
3.4 Experimental Results

This section will outline the complete set of experimental results used in the correlations of Chapter 4, beginning with a discussion of the metal-mold combinations examined. The pertinent features of each experimental result will be discussed, and a comparison to the analytical expressions derived in Section 2.5.1 will be made for each experimental system. Comparison with respect to the current literature and more detailed analysis is contained in Chapters 4 and 5.

3.4.1 EXPERIMENTAL SYSTEMS CONSIDERED

To facilitate the primary goal of this study and extend the heat transfer-air gap correlation to a wide variety of metal-mold systems, the following combination of metals and molds shown in Figure 3.26 were examined.

![Figure 3.26: Metal and Mold Combinations Examined](image)

The metals are essentially aluminum alloys, with tin used for comparison purposes. The molds were selected based on their average thermal diffusivities (equal to the mold thermal conductivity divided by the density and specific heat) which ranged from extremely high to very low ($1.1 \times 10^{-4}$ m$^2$/s for copper, $6.8 \times 10^{-6}$ m$^2$/s for molded graphite from lampblack and $6.6 \times 10^{-7}$ m$^2$/s for green sand). Thermal diffusivity determines the type of temperature profile one would expect in the metal and the mold. This profile can range from cases where the casting can be treated as a
lumped mass soon after pouring, as with sand molds, to cases where the gradients in the casting are greater than those in the mold, as with copper molds. Trials with A206 were accompanied by trials with a two-phase alloy, aluminum 4wt% copper (similar to A206), for comparison. The surface roughness of the molds was estimated as 1.5 µm for copper, 5 µm for graphite, and 500 µm for sand [14-16]. Appendix II lists the set of thermo-physical properties for all materials, including the emissivities of the metals and molds from a number of references [10-12]. Hardness values were not needed for the surfaces, since the metal and mold are under low pressure and retract from each other upon solidification. The order of the alloys used in the experiments was as follows.

<table>
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<tr>
<th>Table 3.3: Order of Experimental Trials</th>
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Significant difficulties were encountered in measuring the air gap formation in sand molds. The LVDT connecting rods could not be adequately placed on the mold inner surface due to the non-uniformities in composition and density existing at the sand interface, and a lack of a proper
CHAPTER 3: EXPERIMENTAL STUDY AND ANALYSIS

binding mechanism to keep the rod at the mold inner surface throughout the casting process. As a result, the air gap measurement curves did not track the air gap formation properly. The trials in sand were consequently used as an application for the completed model, and are discussed in Chapter 5.

3.4.2 THE ALUMINUM-GRAPHITE SYSTEM

The first system considered was the aluminum graphite system. Many of the modifications discussed earlier were made and finally perfected with this system before pursuing other combinations. The results for pure aluminum trials are shown in Figures 3.27(a) and 3.27(b).

![Figure 3.27(a): Heat Transfer Coefficient and Air Gap Size Measurements for the Aluminum-Graphite System](image_url)

In Figure 3.27(a) a combination plot of the measured variables during the early stages of the casting is shown. The heat transfer coefficient is observed to drop from 2500 W/m²/K to about 250 W/m²/K, as the air gap grows to just under 0.12 mm in size. The data shown is from the start of the air gap formation. If the data had been plotted for earlier times, the heat transfer coefficient was seen to rise to a maximum value shortly before the gap began to form.
Figure 3.27(b): Heat Transfer Coefficient-Air Gap Size Correlation for Aluminum-Graphite System

The reasons for this rise are probably due to transient conditions in the casting soon after pouring. Nevertheless, this data should be ignored, and the change in heat transfer coefficient is subsequently monitored only after the air gap begins to form. For our purposes, the heat transfer coefficient before the gap forms is considered to be constant, since the metal is a liquid in intimate contact with the mold.

Refocusing our attention on the curves in Figure 3.27(a), one notes the inverse relationship between the air gap size increase and the overall drop in the heat transfer coefficient. Initially, the drop in the coefficient is steep during the formative stages of the gap. This suggests that the heat flux from the casting is sharply reduced from the moment the air gap forms at the transition from Stage II to Stage III (see Section 2.5.1). Subsequent increases in the air gap size continue to decrease this heat flux, but not with the same intensity as at the moment of initial formation. This observation makes perfect sense, since the extreme insulating nature of air will naturally show an immediate jump in resistance to heat flow through the gap, even at very small thickness, a slower increase in resistance with a change in thickness during Stage III.
In Figure 3.27(b) the magnitude of the heat transfer coefficient is plotted against the size of the air gap, and the analytical solution for a perfectly flat interface based on Equation 2.40 is shown for comparison. The analytical expressions adopt the temperature varying thermal conductivity of air [13] and the emissivities of each metal and mold surface (see Appendix II). The experimental curve can be broken into three zones of different slope: Stages II to IV. Stage II involves a sharp drop in heat transfer coefficient before the air gap has begun to form. Resistance to heat flow increases greatly despite no appreciable gap formation. Here, the contact heat transfer coefficient term \( h_{\text{contact}} \) in Equation 2.33 can be though to be progressively decreasing. Equation 2.40 for perfect surfaces approaches infinity as the air gap approaches zero. For real surfaces, this limit is never reached, and the roughness present between real surfaces will prevent Equation 2.40 from predicting a representative value for the heat transfer coefficient. The transition from Equation 2.33 to 2.35 for a real surface will occur not at an instant, but over a range, which can be observed as a change in the slope of the curve in Figure 3.27(b), as the air gap grows from a minute size to about 0.06mm. This transition zone represents Stage III.

During Stage III, it is believed that two competing factors are most influential in altering the magnitude of the heat transfer coefficient at the interface: the thickness of the air gap, and the degree of surface roughness relative to the air gap size. The air gap size has an inverse effect on the heat transfer coefficient, and the roughness has an effect that is strongest at extremely small gap sizes, and diminishes as the gap size becomes larger. This trend is evident in Figure 3.27(b) as the difference between experimental and analytical solutions is seen to diminish with increasing air gap size.

The curve appears to enter Stage IV at larger gap sizes (>0.06mm). The ‘roughness aspect ratio’ (the size of the surface roughness peaks relative to the magnitude of the air gap) no longer changes as drastically, as it did when the air gap size approached zero. Thus, the transient effect of roughness becomes more and more negligible for larger gap sizes as the surfaces behave more and more as ‘perfectly flat’ surfaces. If the air gap continues to grow, it will eventually reach a magnitude where the roughness of the surfaces can be neglected, and Equation 2.36 can be used to estimate the heat transfer coefficient more accurately. The present study will concern itself with characterizing the heat transfer coefficient at times when the surface roughness cannot
be neglected. Roughness effects are characterized in Chapter 4. The three-zone change in slope pattern has also been observed by other researchers, Gunasegaram [7] and Bellet [8], in other metal-mold systems. For each correlation plot in this study, the slope of the curve during Stage II is greater than during Stage III, which in turn, is greater than during Stage IV.

Although the coupling strategy in this study requires only values of the heat transfer coefficient for implementation, a look at the overall heat flux from the mold wall would prove useful in predicting the cooling rates without the use of a numerical simulation. The heat flux at the mold wall can be calculated with the basic expression:

$$ q'' = h\Delta T $$

(3.15)

where $q''$ is the heat flux of interest, $h$ is the instantaneous heat transfer at the metal-mold interface, and $\Delta T$ is the temperature difference between the metal and the mold surfaces. Figure 3.28 below is a plot of this heat flux as a function of time derived by using the same heat transfer

![Heat Flux Variation during Casting for Aluminum-Graphite System](image-url)
coefficient data in Figure 3.27(a) multiplied by the instantaneous temperature difference between the metal and mold surfaces.

With this plot, the drastic change in the cooling conditions during casting can be appreciated. The flux at early times is extremely high, as both the heat transfer coefficient and the temperature difference are high. At later times, since both the heat transfer coefficient and temperature difference drop, the overall flux falls off remarkably fast. This observation has implications with respect to the grain structure one expects to see at various times during the casting process.

**3.4.3 THE A356-GRAPHITE SYSTEM**

Figure 3.29 shows the accompanying trials using an aluminum alloy, A356, as the casting metal for the same graphite mold.

![Figure 3.29(a): Heat Transfer Coefficient and Air Gap Size Measurements for A356-Graphite System](image)

A356 exhibits different solidification/air gap formation behavior than pure aluminum, and most of that behavior difference can be attributed to the existence of a mushy zone, and to the fact that A356 experiences less thermal contraction than pure aluminum. The gap in A356 resembles the
gap formation in pure aluminum, although its overall magnitude is less than that of pure aluminum due to the smaller coefficient of thermal expansion, and shorter duration time for the experiment. The drop in heat transfer coefficient, from about 1700 Wm⁻²K⁻¹ to 400 Wm⁻²K⁻¹, also occurs more slowly in A356. Because A356 will remain in a mushy state well below the temperature where pure aluminum will be completely solid, it is expected, due to the differences in solidification mechanisms between alloys and pure materials, that the gap may form in a slightly different manner.

The direct correlation in Figure 3.29(b) also exhibits the stages evident with pure aluminum.

![Heat Transfer Coefficient-Air Gap Size Correlation for A356-Graphite System](image_url)

**Figure 3.29(b): Heat Transfer Coefficient-Air Gap Size Correlation for A356-Graphite System**

The experimental error observed with this system is significantly higher than in the pure aluminum-graphite system, which could explain the more ‘distorted’ shape of the curve during Stage III. Once more, the experimental data records a lower heat transfer coefficient than predicted by the analytical expression and again the difference between the curves decreases as the relative effect of roughness diminishes at larger gap sizes. Although most of these similarities
are evident, some definite differences do come into play. The differences include a less steep drop during Stage II, and a higher overall heat transfer rate at later times (since the air gap size is smaller). The less steep drop in Stage II is probably due to the fact that the metal-mold interface for alloys exhibits and maintains a higher Stage II contact resistance.

Figure 3.30 reveals that the heat fluxes observed in A356 are not initially as high as those in pure aluminum (0.18 MW vs. 0.48 MW), since the thermal diffusivity of A356 is less than that of pure aluminum.

![Figure 3.30: Heat Flux Variation During Casting for A356-Graphite System](image)

The overall fluxes at later times are comparable, owing to the fact that the air gap size remains smaller. Overall, one can expect the average cooling rate to be of the same order of magnitude.

### 3.4.4 THE TIN-GRAPHITE SYSTEM

As a low temperature analogue to our aluminum systems, tin served as a comparison metal; to further test our experimental setup. Tin was the only non-aluminum casting material examined, chosen for its tendency to form small air gaps as seen in Figure 3.31.
Figure 3.31(a): Heat Transfer Coefficient and Air Gap Size Measurements for Tin-Graphite System

The large degree of scatter in the air gap data indicated that the accuracy limit of the LVDT was being approached. Notwithstanding this scatter, upon closer examination, one is able to distinguish the stages here as well, in the close up plot of Figure 3.31(c). The size of the air gap remains small so only Stages II and III are observed. The analytical curve (Stage IV) is hence completely inadequate in predicting the heat transfer coefficient, as is obvious from Figure 3.31(b).

Note that the general pattern of heat transfer coefficient drop, from about 900 Wm$^{-2}$K$^{-1}$ to 200 Wm$^{-2}$K$^{-1}$, is very similar to that observed during Stage II and III with A356 and even pure aluminum (although the magnitude of the heat transfer coefficient is much lower, due to the lower thermal diffusivity of tin). The formation of the air gap in tin may well be similar to the air gap formation with aluminum castings, however, LVDTs with more precision would be needed to verify this comparison.
CHAPTER 3: EXPERIMENTAL STUDY AND ANALYSIS

Figure 3.31(b): Heat Transfer Coefficient-Air Gap Size Correlation for Tin-Graphite System

Figure 3.31(c): Close Up of Heat Transfer Coefficient-Air Gap Size Correlation for Tin-Graphite System
The plot of heat flux variation for pure tin in Figure 3.32 shows good relative stability indicating that our thermocouple measurements are relatively stable at lower temperatures.

![Graph of Heat Flux Variation for Pure Tin](image)

Figure 3.32: Heat Flux Variation during Casting for Tin-Graphite System

Again the shape of the flux variation curve is similar to the aluminum-based systems, although at a substantially lower magnitude. For our purposes, the experimental work with tin verifies that the data acquisition system is capable of identifying general trends, even when the accuracy of the system is challenged. This allows us confidence in the results for systems where accuracy is less of a concern.

3.4.5 THE ALUMINUM-COPPER SYSTEM

Before any experiments were conducted with a copper mold, substantially higher cooling rates than those in the graphite mold experiments were expected. Copper was specifically selected, since it represented the highest thermal diffusivity of all commonly used molds in industry. For this reason, it was decided that the aluminum metal-copper mold system would be used to carry out error analysis with multiple samples for both our thermal and mechanical measuring systems. Because the cooling rates in copper were extremely high, any errors in our thermocouple and our
LVDT measurements would have the highest magnitude. In this way, the aluminum-copper system would represent the worst case scenario, and any tolerances for experimental error that were established with this system (see Section 3.2.1) would be higher than the error expected in other systems tested. It was decided to run three trials with this system in an attempt to quantify the worst case error. The three trials were conducted in the identical manner as all previous and subsequent trials in the study. In the first trial, shown in Figure 3.33(a), one can appreciate the change in cooling conditions from the rates seen with graphite molds.

![Graph](image)

**Figure 3.33(a): Heat Transfer Coefficient and Air Gap Size Measurements for Aluminum-Copper System, Trial I**

The growth of the air gap is extremely quick, and the drop in heat transfer coefficient is equally rapid from about 5500 Wm⁻²K⁻¹ to 500 Wm⁻²K⁻¹. Within about 25 seconds after the air gap begins to form and grow, the heat transfer coefficient has dropped by nearly an order of magnitude. This fact has enormous implications, as the formation of the air gap in copper molds contributes more strongly to the reduction in the initial heat transfer coefficient within a short time, a reflection of the higher ratio between the thermal diffusivities of the copper mold and air. Since the grain structure profile of a casting is highly dependent on the cooling rate at the time of
solidification, a drop in heat transfer coefficient can contribute to a transition in structure. The chill crystals, which typically form at the beginning of the casting process at high cooling rates, will give way to columnar crystals as the cooling rate drops. In a similar fashion the effectiveness of adding copper chills to reduce hot tearing effects will be substantially reduced as a gap forms between the copper chill and metal wall.

In Figure 3.33(b), the difference between experimental data and the analytical expression is drastically reduced, compared with the graphite mold trials.

![Graph showing heat transfer coefficient vs. gap size](image)

**Figure 3.33(b): Heat Transfer Coefficient-Air Gap Size Correlation for Aluminum-Copper System, Trial I**

This is a logical observation, since the average roughness of polished copper (1.5 μm) was over an order of magnitude smaller than the average roughness of the graphite (20 μm). The experimental data generally overestimates the analytical estimate and the difference diminishes with air gap size. The analytical estimate, however, is still higher as the limit of zero gap size is approached. The experimental curve of Figure 3.33(b) shows a smoother transition between the three stages than that observed with the graphite molds.
The heat flux variation curve shown in Figure 3.34 below clearly illustrates this rapid drop in overall heat flux.

![Heat Flux Variation Graph](image-url)

**Figure 3.34: Heat Flux Variation during Casting for Aluminum-Copper System, Trial I**

The second trial conducted in the aluminum-copper system shows similar results. The characteristic steep heat transfer coefficient drop and sharp air gap formation rise occurs again over a similar time frame, and the correlation in Figure 3.35(b) is (within the tolerances defined in Section 3.2.1) nearly identical to trial I, as is the flux variation plot in Figure 3.36.

The second set of results indicates that the two experimental trials produced highly repeatable data. A third trial showed similar results, although a slight inflection in the air gap formation curve was recorded, perhaps caused by sticking between the metal and the mold during the early stages of thermal contraction. Despite this blip, the curves in Figure 3.37(b) showed no significant variance from the previous correlations and shared the same trends in relation to the analytical curves.

The heat flux curve was very smooth and comparable to the earlier trials as in Figure 3.38 below. The three trials conducted in the aluminum-copper system are plotted on the same graph in
Figure 3.35(a): Heat Transfer Coefficient and Air Gap Size Measurements for Aluminum-Copper System, Trial II

Figure 3.35(b): Heat Transfer Coefficient-Air Gap Size Correlation for Aluminum-Copper System, Trial II
Figure 3.36: Heat Flux Variation during Casting for Aluminum-Copper System, Trial II

Figure 3.37(a): Heat Transfer Coefficient and Air Gap Size Measurements for Aluminum-Copper System, Trial III
Figure 3.37(b): Heat Transfer Coefficient-Air Gap Size Correlation for Aluminum-Copper System, Trial III

Figure 3.38: Heat Flux Variation during Casting for Aluminum-Copper System, Trial III
Chapter 4, and the differences between the trials indicated very good repeatability. Thus, concerns of whether the results produced via separate experiments are symmetric and repeatable can be safely dismissed.

### 3.4.6 The A356-Copper System

Similar differences to those observed between A356 and pure aluminum cast in graphite molds were also evident between the same metals in copper molds. The LVDT appeared to monitor a very slow air gap formation with less of a plateau after the first 200 seconds as in Figure 3.39.

![Figure 3.39(a): Heat Transfer Coefficient and Air Gap Size Measurements for A356-Copper System](image)

This difference may again be attributed to the mushy zone effect in alloys, and higher error than in the pure aluminum-copper system. The slightly lower heat transfer coefficients ($h_{\text{max}} = 3200 \text{ Wm}^{-2}\text{K}^{-1}$ to $500 \text{ Wm}^{-2}\text{K}^{-1}$ over the first 50 seconds of the experiment) are primarily due to the difference in thermo-physical properties between the metals (the thermal diffusivity of A356 is less than that of pure aluminum). A slight upward bias in the heat transfer coefficient curve of Figure 3.39(a) and the correlation of Figure 3.39(b) were seen for each of the alloys cooled in
copper molds. This upward bias was initially suspected to be experimental error associated with the rapid cooling of alloys, which occurred in copper molds and not in graphite. The reasons for this occurrence cannot be determined conclusively at this stage, but subsequent experimental trials in other alloys, A206 and aluminum 4wt% copper, also exhibited this bias. The experimental data points are lower than the analytical estimate by a greater amount with A356 as compared to pure aluminum, and again the error diminished with increasing gap size. Agreement with the analytical curve was excellent at larger gap sizes. The heat flux plot, shown in Figure 3.40, exhibits no upward bias, and for A356 a characteristic smooth curve is produced. Note the reduction in flux for A356 as compared to aluminum for the early stages of casting. The values shown in this plot correspond well with the maximum value of 2 MW/m² reported by a similar study (Kumar [9]) which calculated the flux for an Al 13.2%Si alloy cast in a copper mold.

3.4.7 THE A206-COPPER SYSTEM
The A206-copper system and the aluminum 4wt% copper alloy-copper system differ only by a few trace elements (the composition of all alloys used in this study are given in Appendix II). The
Figure 3.40: Heat Flux Variation during Casting for A356-Copper System

correlation plots below for A206-copper show a smooth LVDT curve and a good correlation, although the slight amount of upward bias mentioned earlier is detected at higher times.

Examining the analytical curve reveals the same decreasing discrepancy with air gap size seen with other aluminum alloys. The shape of the curve is very close to that of the A356-copper system results, with a lower maximum heat transfer coefficient of about 2400 Wm⁻²K⁻¹ and a slightly lower heat transfer coefficient of 400 Wm⁻²K⁻¹ at an air gap equal to 0.1 mm.

The flux plot exhibits the lowest overall flux of all the aluminum alloys (less than 2 MW), indicative of the lowest thermal diffusivity among the alloys, but as expected, still far higher than any of the graphite mold results.

**3.4.8 THE 4wt% COPPER ALUMINUM-COPPER SYSTEM**
The final trials were conducted with an aluminum 4wt% copper alloy, which is essentially identical to the A206 alloy minus some trace elements. All the curves for this system are near duplicates to the curves plotted for the A206-copper system, although a little bit more scatter is
Figure 3.41(a): Heat Transfer Coefficient and Air Gap Size Measurements for A206-Copper System

Figure 3.41(b): Heat Transfer Coefficient-Air Gap Size Correlation for A206-Copper System
Figure 3.42: Heat Flux Variation during Casting for A206-Copper System

Figure 3.43(a): Heat Transfer Coefficient and Air Gap Size Measurements for 4wt%Cu Aluminum-Copper System
The immediate conclusions that can be drawn from analyzing the preceding curves are that based on both thermocouple and LVDT data, it becomes difficult to distinguish all the systems independently. The differences between the molds are obvious, as are the differences between the tin, pure aluminum, and aluminum alloys. However, the differences between the alloys within the same mold system are nearly impossible to detect. Thus, it becomes very difficult to distinguish the A356 from the A206 data results simply by examining the heat transfer coefficient or heat flux curves. The LVDT can aid in making the distinction, but the overall correlation curves cannot be independently identified from the magnitude of scatter which is evident in the data acquisition system.

The effect of surface roughness on the overall heat transfer coefficient is of paramount importance. The greater the roughness, the greater the drop in heat transfer coefficient (see Section 4.5 for the estimated effect of extremely high roughness in a sand mold). As the size of
the air gap increases the effect of roughness decreases. The thermal diffusivities of the metal and the mold are also seen to play a significant role in determining the magnitude of the heat transfer coefficient. The larger the thermal diffusivity of the metal, the higher the heat transfer coefficient. Similarly, the larger the thermal diffusivity of the metal, the higher the heat transfer coefficient.

More on this topic is contained in Chapter 4.

3.5 Check for Consistency of Results

Before proceeding with a description of the correlation technique in Chapter 4, a strategy for testing the validity of the early trials will be presented.

3.5.1 ENERGY BALANCE CHECK

The heat transfer coefficients calculated above were validated using an energy balance check. In designing an efficient experimental set up, a tool was needed to spot any trial errors immediately after they occurred. Otherwise, one would have had no recourse in differentiating seemingly good data from truly good data, which would have made the correlation stage problematic. The
check employed involves knowing the initial minus the final energy state of the casting plus any latent heat released, i.e.

$$\text{Energy}_{\text{total}} = mC_p(T_{\text{avg, fin}} - T_{\text{init}}) + mL_f$$  \hfill (3.16)$$

and, comparing this value to the sum of the incremental heat losses predicted by the calculated heat transfer coefficients at each recorded experimental increment:

$$\text{Energy}_{\text{total}} = \sum_{t=t_0}^{t_{fn}} q_{\text{incr}} \Delta t$$  \hfill (3.17)$$

where $$q_{\text{incr}} = h_{\text{inst}} A_{\text{sur}} (T_{\text{met, int}} - T_{\text{mold, int}})$$  \hfill (3.18)$$

This process is outlined schematically in Figure 3.45.
The value of the sensible heat would include the energy associated with the superheat of the liquid and the value for $C_p$ would represent the average specific heat of the material between the initial and final states. Since this technique is approximate itself, especially when estimating the average temperature of the casting, trials which differed significantly from the balance energy predicted (the early developmental trials) were suspected to be erroneous, and the experimental setup was modified accordingly. This scheme was invaluable during the development stages.

### 3.5.2 Implementation of the Experimental Technique

The relationships developed in this study qualitatively illustrate the effect of air gap formation on the amount of heat that flows out of the casting. But, the experimental information obtained in this study on its own is not enough to improve the simulation of castings. The information has to integrated into a 'coupling mechanism' from which a numerical algorithm can draw relevant information on a real-time basis. The experimental study addresses the first two parts of this 'coupling mechanism' as illustrated in Figure 3.46. Although invaluable on its own, the preceding experimental work requires a mathematical description of the correlation to be truly practical. This is the focus of Chapter 4.
Chapter References

Correlation Development

The proposed form of the correlation is discussed and regression analysis is conducted on data from the experimental work and the literature. Dimensional analysis is used to generalize the correlations.

The correlation of heat transfer coefficient measurements with air gap formation data was a complicated task. Firstly, it was recognized that much data of this type could already be found in the literature. Studies monitoring the formation of an air gap have been conducted in the past in conjunction with thermocouple measurements at the interface; however, in many cases the authors failed to correlate the two variables. This created a good source of data which could be used to develop correlations without having to conduct new experimental trials. Much of this information, however, was limited to a small number of data points. Consequently, data obtained from experimental work in this study was needed to formulate more comprehensive correlations, and provide further support for the form of the proposed equations.

Before the form of the relationship could be established conclusively, it was necessary to properly define the entire realm of parameters that could influence the correlation. This definition is considered in the next section.

4.1 Background Information

The subject of calculating the heat transfer at the mold metal interface has been oversimplified greatly in much of the literature, much to the detriment of many working in this area. Many of the discrepancies found among different studies can often be attributed to differences in
experimental parameters not included as influencing factors. A more general approach is needed to better unify the work in this field. Weckman [9] gave an excellent review of this subject area.

The heat transfer coefficient at the metal-mold interface of a solidifying casting contracting from the mold wall is a function of several parameters as shown in Figure 4.1.

\[
HTC(x,y,z) = \text{Function} \left[ A, TP_{\text{metal}}, TP_{\text{mold}}, TP_{\text{gas}}, R_{\text{int}} \right]
\]

Figure 4.1: Most Significant Variables Affecting the Heat Transfer Coefficient at the Metal-Mold Interface During Casting

The width of the air gap is the most dominant variable, and has been stressed up to this point. Additionally, the thermo-physical properties of the metal and the mold can affect the equivalent heat transfer coefficient in two ways. Firstly, the metal and mold thermo-physical properties influence the temperature of the metal and the mold interfaces at any given time during solidification. The temperatures of these interfaces can affect the thermophysical properties of the gas in the gap causing heat to flow out of the mold at different rates. Secondly, a change in surface temperatures will influence the rate at which heat is lost via radiation. This effect will become increasingly influential only at higher temperatures, since heat flux due to radiation varies to the fourth power of temperature. The effect of thermo-physical properties on the proposed general correlation is discussed in detail in Section 4.5. Radiation constitutes a maximum of about
5% of the overall heat transfer coefficient value in aluminum castings and far less in tin, so it can safely be neglected in these systems. The thermo-physical properties of the gas in the gap (or more importantly, the conductivity) will greatly influence the heat transfer coefficient, as heat will conduct through the gap from metal to mold surface. The influence of this variable is not explored in the present study, since all of the work is conducted with a single gap gas: air. The thermo-physical property variation of air with temperature, however, is considered.

The metal-mold interfacial roughness, a measure of the initial roughness of the mold inner wall prior to casting, will further effect the heat transfer coefficient. Initially, when the mold and metal surfaces are in contact, the roughness of the metal-mold walls can add considerably to the equivalent resistance of the interface. After a gap begins to form, roughness will still have an important effect, as rough 'peaks' jutting out of either the metal or the mold will act as fins, distorting the paths available for the flow of heat. This effect is accounted for in Section 4.5.

Other variables which can generally influence the heat transfer coefficient (but can be neglected in the metal-mold systems examined in this study) include the emmisivities and hardness of the mold and metal walls, and the pressure at the metal-mold interface. The emmisivities become influential in higher temperature systems, such as steel castings, where the radiative component of the heat transfer coefficient is significant. The hardness of the metal and mold walls, and the pressure at the interface will become influential only in cases where the mold and metal surfaces contract towards each other (i.e., at mold cores) and no air gap forms.

Though the magnitude of the air gap size undoubtedly plays a dominant role in determining the overall heat transferred from metal to mold (since it represents the greatest single source of resistance), neglecting the effect of the other variables can render comparative studies ineffective. Casting in a hydrogen environment, for example, instead of air can increase the heat transfer coefficient four-fold, as noted by Campbell [1]. Indeed, a patent already exists for this process. Whereas unwanted variables can be kept constant for a particular trial, a set of correction factors are needed to extend results to other systems where these variables change significantly. These general considerations will also be examined in Section 4.5.
4.2 Correlation of Experimental Data

Having established the most general form of the equation for the heat transfer coefficient at the interface as:

\[ HTC = \text{function [ air gap size, roughness of mold surface, conductivity of gas in the gap, thermo-physical properties of the metal, thermo-physical properties of the mold, emissivity of the metal and mold walls, hardness of the metal and the mold, contact pressure at the metal-mold interface]} \]

(4.1)

and, by neglecting the variables that are not influential for low temperature (<800°C) casting process where a gap forms, reduced this equation to:

\[ HTC = \text{function [ air gap size, roughness of mold surface, conductivity of gas in the gap, thermo-physical properties of the metal, thermo-physical properties of the mold]} \]

(4.2)

a specific functional form for the relationship can be formulated to correlate both experimental data from the present study, and data available in the literature. Unfortunately, the literature data did not include all of the essential variables of Equation 4.2 for comparison. As a result, the correlations developed in this chapter will adopt a semi-empirical relationship based on the dominant variable of interest, the air gap size. The relationship will allow comparisons to be made between a wide variety of studies. Section 4.5 will present a more general analysis based on the complete set of defined variables in Equation 4.2. The form of the equation was chosen as:

\[ HTC = \frac{1}{k \cdot A + r} + C \]

(4.3)

Though partially empirical, Equation 4.3 can be used to bridge the void in estimating HTC between Stages II and IV described by Equations 2.58-2.61 in Chapter 2. Since Stage III cannot be mathematically defined, Equation 4.3 serves to approximate the transition between Stage II and IV by approaching Equation 2.58 for Stage II as \( A \) approaches 0, and Equation 2.61 for Stage IV as \( A \) approaches infinity. The equation accommodates the dominant air gap size
variable, and allows for variations in roughness, radiation, and other uncontrolled variables present between differing literature studies to be 'absorbed' by the k, r, and C constants. The greater the effects of these variables, the more the constants k, r, and C will differ from trial to trial.

The variables k, A, r, and C are input with the units W⁻¹m²Kmm⁻¹, mm, W⁻¹m²K, and Wm⁻³K⁻¹, respectively. The coefficients r and C can be negative in the correlation, since these values represent the 'calibration' parameters used to fix the inverse relationship to its maximum (initial) and minimum (final) values. The coefficient k must never be negative, since this parameter determines the influence of an increase in air gap size on the resulting heat transfer coefficient. A negative k value would imply the heat transfer coefficient is increasing with an increase in air gap size.

4.2.1 EFFECT OF SECONDARY VARIABLES
Other forms for Equation 4.3 were examined to determine their effectiveness. The correlation equation was modified as in Equations 4.4–4.7, and the data chosen for the new regressions was taken from the pure aluminum casting trials in copper molds. The aluminum-copper system was chosen since the most data was available in this system, having measured 3 separate trials for comparison.

Firstly, however, a preliminary test was conducted to determine the soundness of Equation 4.3. A second-order air gap width term was introduced into Equation 4.3 such that the resulting form of the equation would be

$$HTC = \frac{1}{b \cdot A^2 + k \cdot A + r} + C$$  \hspace{1cm} (4.4)

The inclusion of this second-order term could only result in an improvement in the overall correlation coefficient, since for b=0 the correlation would be identical to Equation 4.3. The results from the regression analysis were convincing, as the overall correlation coefficient improved minusculely from 0.9436 to 0.9477 for the aluminum-copper system. Since one would expect the experimental scatter in the system to have at least this effect, if not more, it was concluded that the addition of this term had no effect on the accuracy of the correlation and
hence could be omitted. This result was expected since the magnitude of the heat transfer coefficient, from the analytical expressions, should only be proportionately related to the thickness of the gap. However, it was still rewarding to see that the regression analysis confirmed this relationship. Armed with this knowledge, the current form of the correlation was tested with respect to the two other measured variables.

The effect of mold and metal temperatures on the heat transfer coefficient could be examined by including two proportionality terms in Equation 4.5

\[ HTC = \frac{1}{k \cdot A + r} + C + d \cdot T_{\text{metal.int}} + e \cdot T_{\text{mold.int}} \]  \hspace{1cm} (4.5)

These terms would serve to substantially improve the correlation if the temperatures at the metal and the mold had a definite effect on the heat transfer coefficient. Even if the effect was of a higher than first-order linear, the inclusion of these terms would still show an appreciable change. The regression analysis performed using Equation 4.5 revealed little improvement, as the correlation coefficient scarcely changed from 0.9436 to 0.9455. The conclusion to be made here, however, must be taken in the proper context. This analysis did not conclusively rule out the possibility that the mold and metal interfacial temperatures had an effect on the heat transfer coefficient. It simply concluded that the effect was very small in comparison to the air gap growth, so small, in fact, that the resolution of the experimental apparatus was practically unable to distinguish the effect from the experimental scatter. Therefore, direct temperature effects will be neglected for the remainder of this work.

An additional correlation equation derived from a combination of terms from Equations 4.4 and 4.5 was fitted to be certain that neither of these effects were indeed valid. This correlation, shown below, was the most complex equation fitted to the experimental curves.

\[ HTC = \frac{1}{b \cdot A^2 + k \cdot A + r} + C + d \cdot T_{\text{metal.int}} + e \cdot T_{\text{mold.int}} \]  \hspace{1cm} (4.6)

The improvement in the fit was again negligible, as the new correlation coefficient rose minutely from 0.9436 to 0.9479, and thus the exclusion of both terms was justified.
A final modified equation was used to test the variability of the thermophysical properties of the gas at the interface. The simplest way to achieve this was via the equation

\[ HTC = \frac{1}{k \cdot (1 - \text{metal}_{\text{int}}) \cdot A + r} + C \]  

(4.7)

where even though the exact nature of the gas' change in thermophysical properties with time were not known, they were assumed to be a function of temperature, and allowed to vary accordingly in Equation 4.7. Thus a change in properties with temperature would simply result in a different value for the coefficient \( k \) to account for this effect. The resultant analysis revealed that there was actually a drop in the correlation coefficient from 0.9436 to 0.9329. Consequently, the effects of variable gas diffusivity was again at least an order of magnitude less than the air gap width, and of the same range as the experimental variability.

As a result of the dominance of the air gap size in predicting the overall heat transfer coefficient, the inclusion of additional variables in the calculation scheme is unwarranted. The semi-empirical correlations become significantly more complex, and as the law of diminishing returns dictates, the increased amount of effort results in a negligible improvement for this situation. Furthermore, in an industrial setting, away from the controlled conditions of the laboratory, some of these additional variables are nearly impossible to measure accurately. In applying many techniques, the simplest solution is often the most effective, and in this case this statement is very true.

### 4.2.2 EFFECT OF COATINGS/WASHES

In industrial castings, a coating or wash is often applied to the mold inner surface for a number of reasons as described by Kaiser [8]: to control the chill rate, to minimize thermal shock and/or to prevent sticking between the cast metal and the mold wall. With respect to the interfacial heat transfer coefficient, a coating will generally impede the flow of heat from the metal casting to the mold. The thicker the refractory wash, the more the resistance to heat flow, and the lower the heat transfer coefficient. A graphite coating is often used when a sharper reduction in the chill rate is not desired.
A coating or wash can thus be viewed as a mold with an additional barrier to heat flow, or simply a mold with different thermophysical properties. A copper mold with a graphite coating will behave somewhere in between a pure copper and a pure graphite mold. The correlation curve will still exhibit an inverse relationship and a mathematical model of the casting can simply assign the mold control volume adjacent to the interface a different set of thermophysical properties conforming to those of the coating.

The next sections will outline the correlation performed with data from this study. A discussion of the pertinent features, relative differences, and comparisons to an analytical expression were given in Chapter 3.

4.2.3 PURE ALUMINUM CAST IN A GRAPHITE MOLD
No work exists in the literature describing measured heat transfer coefficients in graphite, let alone a heat transfer coefficient-air gap correlation, so our experimental work in this area is unique. The original data from the experiment is shown in Figure 4.2.

![Figure 4.2: Correlation Plot for Commercial Purity Aluminum Cast in a Graphite Mold](image-url)
The inverse curve fit the data quite well. At earlier times the experimental data showed a negative bias with respect to the curve, at later times the bias is positive, but eventually the curve and the data points approached a similar value. The three stages observed experimentally (see Stages II, III, and IV in Section 2.5.1) are satisfactorily represented by one curve with less than 15% maximum error. The values of the k, r, and C are shown in Figure 4.2. Note that the value of k obtained in this system will be the same order of magnitude as most of the subsequent correlations for other systems. This indicates that the general value for k is closely tied to the thermal conductivity of the gas in the gap. As A approaches zero in Equation 4.3, the value of the heat transfer coefficient approaches 1760 Wm⁻²K⁻¹ (the equivalent value of \( h_{\text{conv}} \) in Equation 2.58). At larger values of A, Equation 4.3 will approximate the first term in Equation 2.61, as the relative effect of r and C are reduced for increasing values of A.

### 4.2.4 A356 ALUMINUM ALLOY CAST IN A GRAPHITE MOLD

The correlation with A356 in a graphite mold was the least conventional. The shape of the curve, and the extremely low value of k indicates that, despite the good correlation coefficient, the
inverse relationship has less curvature than would be expected. The fit is shown in Figure 4.3.
The curve predicts a heat transfer coefficient of 1631 Wm⁻²K⁻¹ as A approaches zero \( (h_k = 1631 \text{ in Equation 2.58}) \), which is reasonable, but only approaches Equation 2.61 as A grows to 2 mm (i.e., the product of kA in Equation 4.3 becomes an order of magnitude larger than \( r \)). Additional trials with this metal-mold system would probably reveal that the actual trend would have less of a linear pattern.

**4.2.5 PURE TIN CAST IN A GRAPHITE MOLD**

Despite the scatter present in the tin-graphite system, the resulting correlation was quite well behaved (see Figure 4.4).

![Figure 4.4: Correlation Plot for Pure Tin Cast in a Graphite Mold](image)

The regression equation had a reasonable \( k \) value and a good correlation coefficient. As \( A \) approaches zero, a value of \( h_k = 775 \text{ Wm}⁻²\text{K}⁻¹ \) is calculated for Stage II, and a value of \( A = 0.1 \text{ mm} \) will result in a dominant kA term, and hence a good approximation for Equation 2.61.
Thus, Equation 4.3 will only approximate Stage II and III behavior with this system. The experiment could be conducted with better precision LVDTs if the correlation is to be used for simulations with more accurate requirements. For the purposes of this study, however, the trend is satisfactorily characterized.

4.2.6 PURE ALUMINUM CAST IN A COPPER MOLD

Up to this point, the trials conducted, although appearing to be reasonable, could not be validated via other work in this field (since no such work had been published). The subsequent trials in pure copper could, however, be compared with similar work. The word 'similar' is used to denote that many discrepancies could be present between two otherwise identical studies due to a lack of standardization in techniques. Some of these discrepancies could relate to the cooling techniques used, lack of one-dimensionality in the system and differing techniques used to obtain heat transfer coefficient data. Nevertheless, most of the studies produced similar correlations. The experimental curve fits for the three aluminum-copper system trials conducted in this study are shown in Figure 4.5.

![Figure 4.5: Correlation Plot for Commercial Purity Aluminum Cast in a Copper Mold](image-url)
As $A$ approaches zero, the Stage II heat transfer coefficient is equal to 462 Wm\(^{-2}\)K\(^{-1}\). Compared to studies conducted by El-Mahallaway [3] and Pehlke [2], illustrated later in Section 4.3.1, the value of $k$ obtained is lower than in both these previous works. The experimentally measured heat transfer coefficient at the beginning of the casting process is similar to that of El-Mahallaway [3], who records a maximum heat transfer coefficient of about 5200 Wm\(^{-2}\)K\(^{-1}\), but higher than the value calculated by Pehlke [2] (2800 Wm\(^{-2}\)K\(^{-1}\)). The values of HTC at the maximum recorded gap size (0.032 mm) in El-Mahallaway’s [3] study, and the present study, are both about 2000 Wm\(^{-2}\)K\(^{-1}\); and the $h$ values at the maximum recorded gap size (0.25 mm) in the present study, and in Pehlke’s [2] study are both about 800 Wm\(^{-2}\)K\(^{-1}\). The comparisons between these studies are made, despite the fact that the size of the castings varied, and hence the magnitude of the air gaps formed ranged from 0.032 to 0.3 to 5 mm (i.e., the studies covered different ranges).

4.2.7 A356 ALUMINUM ALLOY CAST IN A COPPER MOLD

Results in the A356-copper system are shown below in Figure 4.6. The heat transfer coefficient during Stage II given by Equation 4.3 is 2941 Wm\(^{-2}\)K\(^{-1}\), and Equation 4.3 agreed with the

![Figure 4.6: Correlation Plot for A356 Aluminum Alloy Cast in a Copper Mold](image-url)
analytical approximation for Stage IV as A surpassed 0.05 mm. The data agreed very well with the limited data available in the literature for aluminum alloys. The k value of 0.0717 compares favorably with Gunasegaram's [5] value of 0.049 for an Al 7wt% Si alloy with no coating, but is significantly higher than Nishida's [4] 0.0087 k value for an Al 13wt% Si alloy with a graphite coating (see Section 4.3.3 and 4.3.4). The measured maximum heat transfer coefficients in Gunasegaram's [5] and Nishida's [4] trials were 8000 Wm\(^{-2}\)K\(^{-1}\) and 3000 Wm\(^{-2}\)K\(^{-1}\), respectively, placing the data in Figure 4.6 somewhere in between.

**4.2.8 A206 ALUMINUM ALLOY CAST IN A COPPER MOLD**

The correlation for the A206-copper system was similar to that for the A356-copper system with a slightly lower k value of 0.0547 and nearly identical values for the other coefficients. This trial is shown in Figure 4.7 below.

![Figure 4.7: Correlation Plot for A206 Aluminum Alloy Cast in a Copper Mold](image)
The stage II heat transfer coefficient is 2564 Wm⁻²K⁻¹, and Equation 4.3 agrees with Equation 2.61 as A values exceed 0.077 mm for this system. A k value of 0.05 corresponds well with the average k value of 0.0359 from all of the correlations conducted in this study. The studies of Vincente-Hernandez [6], Bellet [7], and Gunasegaram [5] in steel molds (see Section 4.3.5) produced even lower k values of 0.022, 0.0062, and 0.028 respectively.

4.2.9 ALUMINUM 4wt% CU ALLOY CAST IN A COPPER MOLD
The final trial, Al 4wt%Cu cast in a copper mold again showed very little difference from the A206 correlation. Since A206 and Al 4wt%Cu differ only by the addition of some trace elements, the equality in these two correlations can serve the same purpose as the set of three trials in the pure aluminum-copper system—to further validate that the accuracy in the data acquisition system is sufficient.

![Correlation Plot](image)

**Figure 4.8: Correlation Plot for Al-4wt%Cu Aluminum Alloy Cast in a Copper Mold**
CHAPTER 4: CORRELATION DEVELOPMENT

Similar to the A206-copper system, the Stage II heat transfer coefficient is 2941 Wm⁻²K⁻¹, and Equation 4.3 agrees with Equation 2.61 as A exceeds 0.05 mm.

The effect of the alloy composition on the overall k value is seen to be minimal. In fact the results for all three alloy A356, A206 and Al 4wt%Cu are, for all intents and purposes, indistinguishable. In Chapter 5, the preceding correlations will be coupled to a numerical solution algorithm.

4.3 Correlation of Data from the Literature

In conducting a literature survey of work examining the solidification of metals, data was uncovered which could be used to compliment the experimental base of data established in Chapter 3. Admittedly, many deterrents to making a direct comparison between the data existed. Firstly, the data available only considered copper or steel molds, and some of the molds had coatings applied to the mold wall. The geometries of the castings, often indicated that the temperatures used to calculate the heat transfer coefficients were not recorded from a one-dimensional system. Since the techniques used by these studies to calculate heat transfer coefficients rely on uni-directional heat flow, if the system is not one-dimensional, the thermocouples would introduce error caused by cooling in a secondary direction. Also, the alloys used in the studies varied drastically in composition, and the pouring superheat was often not reported. Nevertheless, the overall data trends should follow an inverse relationship qualitatively, and indeed, this was the main purpose for the review. The variance in the calculated coefficients from the literature data was the main indication that the experimental conditions were different in each case. Additional relevant information was rarely available in these studies.

4.3.1 PURE ALUMINUM CASTINGS IN COPPER MOLDS (NO COATINGS)

Only two trials were discovered in the literature documenting both heat transfer coefficients and air gap growth for pure aluminum cast in a copper mold: the work of Pehlke et al. [2] and El-Mahallawy [3]. Neither of these researchers attempted to directly correlate their data. The first set of data shown in Figure 4.9 is from El-Mahallawy's paper [3], for a cylindrical specimen heated in a resistance furnace and cooled via a water chilled copper plate from the bottom end of the cylinder.
The data obtained from this study is examined with respect to the following criteria. Firstly, the positioning of the thermocouples was not ideal for accurately predicting gradients, since thermocouples were not placed close to the interface. Secondly, the stored energy in the furnace acted as a further source of heat during the experiment, and the results may not be comparable to a typical casting operation. Indeed, the authors found a significant change in the heat transfer coefficients, for changes in initial superheat after the air gap had formed, which one would not expect in a typical casting operation, since the metal and mold at the wall would eventually have similar temperatures, and hence similar heat transfer coefficients.

Nevertheless, the data correlated quite well to the inverse equation in Figure 4.9. Since data was available only over a small air gap range (less than 0.02 mm), and relatively far from $A = 0$, the values of $k$, $r$, and $C$ generated for Equation 4.3 were very atypical, and did not properly account for Stage II and IV analytical behavior. The inverse form of the equation will often take into
account differences present in an experimental set up assuming the temperature and position measurements are consistent (although the coefficients obtained for the correlation will not reflect those from a more typical casting situation), and in this case, are only applicable for Stage III. The narrow range of heat transfer coefficient values (5000 Wm⁻²K⁻¹ to 2000 Wm⁻²K⁻¹) are in the range of typical Stage III values observed in Section 4.2.

The second trial conducted by Pehlke [2] et al. rectified some of the problems evident in the El-Mahallawy trial [3], by measuring the heat transfer coefficient and air gap from the top of the casting. His set up behaved more like a one-dimensional system thermally, however, mechanically, the system was subject to frictional forces on the side of the mold wall, which effectively made the air gap measurements more unpredictable, as the metal could stick to the mold wall and hinder the rate of air gap formation.

![Graph showing correlation plot](image)

**Figure 4.10: Correlation Plot from the work of Pehlke [2], Commercial Purity Aluminum Cast in a Copper Mold**
The choppy plot of metal and mold positions given in his paper reflects this behavior. The values of the heat transfer coefficient reported appear to be lower than most studies although Pehlke's data [2] correlates quite well with our proposed equation as shown in Figure 4.10. The study examined the growth of the gap to a size of 5 mm, and the resulting shape of the correlation curve is applicable for Stages II to IV inclusive. The Stage II heat transfer coefficient was 2410 Wm⁻²K⁻¹, far lower than most studies with copper moulds.

4.3.2 PURE ALUMINUM CASTINGS IN COPPER MOLDS WITH COATINGS
The final set of experimental data found in the literature for pure aluminum cast in a copper mold used a 0.01 mm graphite coating on the mold. This coating can change the overall flux at the interface significantly, so this result is not categorized in Section 4.3.1. The experiment was conducted by Nishida [4] and, although the size of the air gap was not even graphed, this value could be obtained from separate plots of the relative positions of the mold and metal.

![Correlation Plot](image)

**Figure 4.11**: Correlation Plot from the work of Nishida [4], Commercial Purity Aluminum Cast in a Copper Mold with 0.01mm Graphite Coating

Correlation Coefficient = 0.9778

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>r</td>
<td>3.63x10⁻⁵</td>
</tr>
<tr>
<td>k</td>
<td>0.046</td>
</tr>
<tr>
<td>C</td>
<td>74</td>
</tr>
</tbody>
</table>
This study was one of the oldest of its kind, but the data correlated again quite soundly. The Stage II heat transfer coefficient is extremely high at 27 548 Wm$^{-2}$K$^{-1}$, a reflection of attempting to use Equation 4.3 across a large air gap range (> 4 mm). Equation 4.3 agrees with Equation 2.61, however, at an A value of only 0.0079 mm or greater.

The heat transfer coefficient values are slightly lower than the norm (3200 Wm$^{-2}$K$^{-1}$ to 200 Wm$^{-2}$K$^{-1}$, as the gap grew to only 0.07mm), and are attributed to the fact that a coating of lower thermal diffusivity than the mold was used.

4.3.3 ALUMINUM ALLOY CASTINGS IN COPPER MOLDS (NO COATINGS)

A single trial using an aluminum alloy in a copper mold was conducted by Gunasegaram [5] in a cylindrical casting with differing radii. Gunasegaram [5] attempted to plot the value of his measured heat transfer coefficients vs. the air gap size, but he used only four points from his experimental results to produced three straight line segments. These segments correspond roughly with the observed stages discussed in the present experimental work. If an inverse

---

**Figure 4.12: Correlation Plot from the work of Gunasegaram [5], Aluminum-Si Alloy Cast in a BeCu (ASTM:C17510) Mold with Insulating Ladle Coat**
relationship curve with the same data as in Figure 4.12 is plotted, the correlation is nearly exact. The Stage II heat transfer coefficient is calculated as 8000 Wm\(^{-2}\)K\(^{-1}\), and Stage IV agreement is reached as \(A\) exceeded 0.026 mm.

Note that the mold used in his study was BeCu, not pure copper. The alloy used in the study was an aluminum 6.71-6.83wt% silicon alloy with less than 1wt% Mg-Cu-Fe and less than 0.05wt% Cr-Ni-Mn-Ti-Sr. Gunasegaram [5] has also published data for a different section cylinder cooled via a steel mold (see Section 4.3.5).

4.3.4 ALUMINUM ALLLOY CASTINGS IN COPPER MOLDS WITH COATINGS

Nishida [4] conducted the identical experiment described in Section 4.3.2, using the same procedure, with an aluminum 13wt% silicon alloy. The corresponding data is shown in Figure 4.13. This correlation produced a Stage II heat transfer coefficient of 4310 Wm\(^{-2}\)K\(^{-1}\), and Equation 4.3 agrees with Equation 2.61 as \(A\) exceeds 0.22 mm.

![Figure 4.13: Correlation Plot from the work of Nishida [4], Aluminum 13wt%Si Alloy Cast in a Copper Mold with 0.01mm Graphite Coating](image)

Correlation Coefficient = 0.9994

\[
\begin{align*}
    r &= 1.93 \times 10^{-4} \\
    k &= 0.0087 \\
    C &= -879
\end{align*}
\]

Regression Equation

Experimental Data Points
4.3.5 ALUMINUM ALLOY CASTINGS IN STEEL MOLDS (NO COATINGS)

Three trials using steel molds were published by three separate authors: Vicente-Hernandez [6], Bellet [7] and Gunasegaram [5]. Vicente-Hernandez [6] used a cylindrical geometry, but placed a water cooled core at the center of the cylinder, in effect creating a tube which solidifies radially outward. The study adopted a heat balance at the interface to calculate the heat transfer coefficient, but in this case heat flow was from the mold to the metal. The results from this experiment again were not correlated by the author, and Figure 4.14 shows a good fit even though the direction of the heat flux was reversed.

![Correlation Plot](image)

**Figure 4.14:** Correlation Plot from the work of Vicente-Hernandez [6], Aluminum 4.5wt%Cu-Mg-Ti Alloy Cast in a Fe-0.14wt% C-0.35wt% Si-1.2wt% Mn Mold

Bellet’s [7] work attempted to use the same experimental set up as Vicente-Hernandez [6] but without the center water-cooled core. This change seriously compromised the one-dimensional flux assumption of Vicente-Hernandez’s [6] work, since the aspect ratio was not sufficient to limit end effects, especially with the relatively long duration of the study. Bellet [7] plotted a
correlation curve of three straight line segments as Gunasegaram [5] did, and the results from his data have been re-plotted in Figure 4.15 with the inverse form of our correlation curve.

![Correlation Plot](image)

**Figure 4.15: Correlation Plot from the work of Bellet [7], Aluminum 7wt%Si-0.3wt%Mg Alloy Cast in a Fe-0.14wt% C-0.35wt% Si-1.2wt% Mn Mold**

Although the set up is nearly identical to Vincente-Hernandez's experiment [6], the absence of the water cooled core resulted in a drastic difference in the k coefficient. The heat transfer coefficients for both of these studies also appear to be quite low. Data for a steel mold was also supplied by Gunasegaram [5]. His measurements recorded an extremely high heat transfer coefficient of 10000 W/m²K at the start of the experiment. This value is in stark contrast with the previous two works by a factor of more than 20. The correlation from this work is given below in Figure 4.16.

To summarize, the range of heat transfer coefficients for steel molds varied from a maximum of 10000 Wm⁻²K⁻¹ to a minimum of 260 Wm⁻²K⁻¹ at zero air gap, and a maximum of 1700 Wm⁻²K⁻¹
Figure 4.16: Correlation Plot from the work of Gunasegaram[5], Aluminum-Si Alloy Cast in a H13 Hot Worked Steel Mold with Insulating Ladle Coat

to a minimum of 220 Wm⁻²K⁻¹ at an air gap size of 0.03 mm. The variance is greater than an order of magnitude, and leaves little consensus among the studies.

At this point it is worthwhile to mention that all of these correlations from the literature were performed with fewer than 10 data points, some with as few as 4, due to incomplete reporting of these numbers from the study. Admittedly, some of these studies did not anticipate further research in this direction, but other studies, presented plots of their own often omitting this essential quantity of data. The regression analysis conducted on the literature data produced very high correlation coefficients, although a higher number of data points could have provided further confidence in the results.

A summary of the experimental results and correlations appear in Table 4.1. The values in bold were obtained from data from the literature. The results from many of these experimental trials
Table 4.1: Summary of Experimental Results and Correlations

<table>
<thead>
<tr>
<th>System metal/mold*</th>
<th>$h_{\text{maximum}}$ [W/m²K]</th>
<th>$h_{\text{minimum}}$ [W/m²K]</th>
<th>Maximum Gap [mm]</th>
<th>Stage II Effectiveness of Equation 4.3 at $A = 0$</th>
<th>Stage III Effectiveness of Equation 4.3 at int. A</th>
<th>Stage IV Effectiveness of Equation 4.3 at large A</th>
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</thead>
<tbody>
<tr>
<td>Al/Graphite</td>
<td>2400</td>
<td>250</td>
<td>0.1</td>
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<td>good</td>
<td>good</td>
</tr>
<tr>
<td>A356/Graphite</td>
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<td>0.04</td>
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<td>poor</td>
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</tr>
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<td>0.05</td>
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<td>Al Alloy/Steel</td>
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<td>Al Alloy/Steel</td>
<td>260</td>
<td>100</td>
<td>0.37</td>
<td>good</td>
<td>good</td>
<td>poor</td>
</tr>
<tr>
<td>[7]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Al Alloy/Steel</td>
<td>10000</td>
<td>1700</td>
<td>0.03</td>
<td>poor</td>
<td>good</td>
<td>good</td>
</tr>
<tr>
<td>[5]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*data in bold indicates values derived from literature data
indicate that the value of heat transfer coefficients and air gap measured can vary substantially from trial to trial, where experimental procedures are not conducted in a consistent fashion. This variance will manifest itself as a change in the coefficients of the heat transfer coefficient-air gap correlation. Thus an experiment run without proper insulation will still behave in a similar manner to an experiment conducted in a media with different thermo-physical properties, i.e. in an inverse fashion. The empirical trend will exist independent of specific variables, which ultimately serve to identify the specific conditions for a particular experimental set up. This observation has also been verified by the experimental work conducted in this project.

4.4 Residual Error

Having presented a series of curve fits in the previous sections, a discussion of residual error is now appropriate. By approximating the data set for each system with a numerical equation, an additional inaccuracy, completely unrelated to experimental error was introduced. This error is termed the residual error, and can be quantified by the correlation coefficient, an approximate measure of the average residual in each system. Appendix IV lists the regression statistics for each correlation in this study. The data from the regression analysis with the aluminum-copper system appears below in Table 4.2.

Table 4.2: Correlation Parameters for 3 Aluminum-Copper System Trials

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
<th>68% (+/-)</th>
<th>90% (+/-)</th>
<th>95% (+/-)</th>
<th>99% (+/-)</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>0.000185343</td>
<td>1.06E-08</td>
<td>1.75E-08</td>
<td>2.12E-08</td>
<td>2.73E-08</td>
</tr>
<tr>
<td>b</td>
<td>2.880329688</td>
<td>0.000734195</td>
<td>0.001208637</td>
<td>0.00146839</td>
<td>0.001890463</td>
</tr>
<tr>
<td>c</td>
<td>-651.0736132</td>
<td>0.258980145</td>
<td>0.426335125</td>
<td>0.51796029</td>
<td>0.666842442</td>
</tr>
</tbody>
</table>

The residuals calculated from each data point can be plotted as in Figure 4.17.
Figure 4.17: Residual Error Plot for 3 Aluminum-Copper System Trials

Note that the data points at earlier times exhibited far greater residual error than the data points, at later times when the air gap size was larger. This trend is in direct contrast to the decreasing experimental error in heat transfer coefficient measurement witnessed for later times. Residual error and experimental error are thus seen to be unrelated to each other. Further evidence of this mutual exclusivity comes from examining the equivalent correlation statistics and residual plot for the tin-graphite system.

Table 4.3: Correlation Parameters for 3 Tin-Graphite System

<table>
<thead>
<tr>
<th>CORRELATION STATISTICS: TIN-GRAFITE SYSTEM (for y = 1/(a + bx) + c)</th>
<th>Confidence interval</th>
</tr>
</thead>
<tbody>
<tr>
<td>Variable</td>
<td>Value</td>
</tr>
<tr>
<td>a</td>
<td>0.0000810619</td>
</tr>
<tr>
<td>b</td>
<td>80.18637858</td>
</tr>
<tr>
<td>c</td>
<td>-457.7971812</td>
</tr>
<tr>
<td>Min Residual</td>
<td>Max Residual</td>
</tr>
<tr>
<td>0.140550397</td>
<td>217.0738521</td>
</tr>
</tbody>
</table>
Now, while the experimental error for the tin-graphite system was seen to be excessive, the residual plots reveal that the maximum residuals are about four times less than the residuals of the aluminum-copper system. This despite the fact that the data showed an apparent scatter that looked to be well above the smoother aluminum-copper correlation curve.

![Residual Error Plot for Tin-Graphite System Trial](image)

**Figure 4.18: Residual Error Plot for Tin-Graphite System Trial**

By examining the correlation statistics and residual plots (Appendix VII) from each system, the following trends were established:

- The residuals for graphite and tin mold trials are generally lower than the residuals for copper mold trials, primarily because the magnitudes of the heat transfer coefficients are lower.

- The residuals are generally larger for earlier experiment data, since the temperature gradients are also higher, but subsequently reduce with time as the gradients drop. This trend was more evident with curve fits possessing a high correlation coefficient.

- The residuals of pure metal trials are generally better behaved than the alloy trials, showing a smoother transition from high to low, irrespective of the mold used.
Thus far, all results have been presented with respect to a particular metal-mold system. Section 4.5 will generalize the results on the basis of the thermo-physical properties of the metal, mold, and the gap gas in the systems examined.

4.5 Dimensional Analysis

Although the correlations presented to this point would be of definite interest to anyone working with the identical metal-mold systems examined in this study, a process change involving the substitution of a different metal or mold would leave one without any relevant data until new experiments could be conducted.

By presenting the results in a dimensionless format, the effects of changing parameters can be anticipated in advance, and a good estimate of the effective heat transfer coefficient can be obtained without further experimentation. The first stage in this process involved identifying the dimensionless ratios applicable for these systems.

4.5.1 DERIVING THE DIMENSIONLESS GROUPS

The variables of interest were identified and discussed in earlier sections and are presented together in Table 4.4. Non-dimensional groups were derived partly by using Buckingham Pi theory, and partly from previous experience with non-dimensional analysis in thermal systems. Firstly, the magnitude of the gap was non-dimensionalized in relation to its ultimate size with the term

$$A^* = \frac{A}{(\text{CTE}_{\text{metal}} \cdot \Delta T_{\text{metal}} - \text{CTE}_{\text{mold}} \cdot \Delta T_{\text{mold}}) \cdot \frac{D}{2}}$$ (4.8)

where $A^*$ represents the non-dimensional size of the air gap. The heat transfer coefficient was encompassed in a dimensionless term derived from the conductive term of the Equation 2.61:

$$h^* = \frac{hA}{k_{\text{gas}}}$$ (4.9)

Thus a decrease in the conductivity of the gas, or an increase in the gap size will cause the
Table 4.4: Variables Used to Form Dimensionless Groups

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$h$</td>
<td>heat transfer coefficient, $W \text{ m}^{-2} \text{ K}^{-1}$</td>
</tr>
<tr>
<td>$A$</td>
<td>size of the air gap, $m$</td>
</tr>
<tr>
<td>$K_{\text{gas}}$</td>
<td>thermal conductivity of the gap gas, $W \text{ m}^{-1} \text{ K}^{-1}$</td>
</tr>
<tr>
<td>$\alpha_{\text{metal}}$</td>
<td>thermal diffusivity of the metal, $m^{2} \text{ s}^{-1}$</td>
</tr>
<tr>
<td>$\alpha_{\text{mold}}$</td>
<td>thermal diffusivity of the mold, $m^{2} \text{ s}^{-1}$</td>
</tr>
<tr>
<td>$\alpha_{0}$</td>
<td>reference thermal diffusivity value (copper at $20^\circ C$), $m^{2} \text{ s}^{-1}$</td>
</tr>
<tr>
<td>$R$</td>
<td>average roughness of the mold, $\mu m$</td>
</tr>
<tr>
<td>$D$</td>
<td>diameter of the cylinder, $m$</td>
</tr>
<tr>
<td>$\text{CTE}_{\text{metal}}$</td>
<td>coefficient of linear thermal expansion of the metal, $K^{-1}$</td>
</tr>
<tr>
<td>$\text{CTE}_{\text{mold}}$</td>
<td>coefficient of linear thermal expansion of the mold, $K^{-1}$</td>
</tr>
<tr>
<td>$\Delta T_{\text{metal}}$</td>
<td>average temperature drop of the metal below solidus, $K$</td>
</tr>
<tr>
<td>$\Delta T_{\text{metal}}$</td>
<td>average temperature rise of the mold above room temperature, $K$</td>
</tr>
</tbody>
</table>

As the thermal diffusivity of the metal or mold increases, the effective heat transfer coefficient will increase, and the non-dimensional term:

$$\alpha^* = \left( \frac{\alpha_0}{\alpha_{\text{metal}}} \right)^m \left( \frac{\alpha_0}{\alpha_{\text{mold}}} \right)^n$$  \hspace{1cm} (4.10)
is defined to account for this dependence. The exponents \( m = 2 \) and \( n = 1/2 \) are found to best correlate the experimental curves. The final dimensionless term is used to normalize the effects of roughness. The term:

\[
R^* = \left( \frac{R}{D} \right)^p
\]

(4.11)

with \( p = 0.12 \) was found to offset the effects of roughness between the copper (\( R = 1.5 \) \( \mu \)m), graphite (\( R = 5 \) \( \mu \)m) and sand (\( R = 500 \) \( \mu \)m) molds.

**4.5.2 DIMENSIONLESS CORRELATIONS**

A plot of data from each of the experiments in this study using the dimensionless ratios \( h^* \) and \( A^* \) is given in Figure 4.19. If the surfaces of the metals and molds were perfectly flat, a plot of \( h^* \) as a function of \( A^* \) would show a simple linear relationship. However, the actual data deviates from this ideal case due to the presence of roughness. The dimensionless term \( R^* \) is used to normalize these deviations and allow for a more accurate comparison of the experimental results.

![Figure 4.19: Dimensionless Plot of h* vs. A*](image-url)
vs. $A^*$ would give a horizontal straight line at a constant value of $h^*$, since analytically $hA = k_{gas} = A$ a constant (assuming the conductivity of the gas changes by a small amount over a small temperature range). Thus, as $A$ increases, $h$ decreases proportionally, and $h^*$ remains constant with increasing $A^*$. An examination of Figure 4.19 reveals that this is indeed the case for larger values of $A^*$, but at smaller gap sizes, the relationship breaks down. The value of $h^*$ drops dramatically, almost by two orders of magnitude for certain systems, as the gap size approaches zero. This extreme drop is caused by the roughness, which exists between real surfaces. As the gap size becomes smaller and smaller, the magnitude of the roughness peaks effectively cause the surfaces to behave less and less 'flat'. Consequently, the analytical approximations break down as the relative size of the gap decreases. Notice that as the air gap grows, the data behaves more and more like the analytical approximation.

Figure 4.20 shows a plot of the product of $h^*$ and $\alpha^*$ vs. $A$. The $\alpha^*$ term has compensated for
the effect of differing mold and metal thermo-physical properties on the magnitude of the heat transfer coefficient. It is expected that the heat transfer coefficient will rise with an increase in either the metal or mold thermal diffusivity. As observed from the experimental data, the coefficients \( m = 2 \) and \( n = ½ \) indicate that the metal diffusivity plays a greater role in increasing the overall heat transfer coefficient.

Finally in Figure 4.21, the plot of \( h*α*R^* \) vs. \( A \) incorporates the roughness correction term \( R \).

![Figure 4.21: Dimensionless Plot of \( h*α*R^* \) vs. \( A \)](image)

Note that all of the data in the plot can now be approximated via a single curve. The choice of \( p = 0.12 \) indicates a moderate change in the effective heat transfer coefficient with roughness. Note that this correction factor is a constant term, representing the average effect of roughness, and will under approximate the correction at lower air gap sizes. This is seen in the aluminum-sand curve, which under approximates the general curve by a high amount at lower gap values. A
correction term as a function of $A$ is needed to account for the diminishing effects of roughness with gap growth, but a function of this type is beyond the scope of this work, and requires further experimentation with more rough surfaces. The range of applicability of the data in Figures 4.19-4.21 is given as:

$$D = 0.06 \text{ m}$$
$$500 \mu m \geq R \geq 1.5 \mu m$$
$$7.5 \times 10^{-5} \text{ m}^2s^{-1} \geq \alpha_{\text{metal}} \geq 4.0 \times 10^{-5} \text{ m}^2s^{-1}$$
$$1.17 \times 10^{-4} \text{ m}^2s^{-1} \geq \alpha_{\text{mold}} \geq 6.6 \times 10^{-7} \text{ m}^2s^{-1}$$
$$0.3 \text{ mm} \geq A \geq 0$$
$$0.06 \text{ Wm}^{-1}K^{-1} \geq k_{\text{gas}} \geq 0.03 \text{ Wm}^{-1}K^{-1}$$
$$700^\circ C \geq T \geq 200^\circ C$$

(4.12)

based on the thermo-physical properties and dimensions of the experimental set up.

**Chapter References**


Numerical Study and Analysis

The implemented numerical model is constructed and a variety of numerical results, including model validations and applications are described.

As suggested throughout all the preceding chapters, the mathematical modeling of the casting process involved firstly identifying the appropriate phenomenon of interest in the process, secondly, determining the governing equations which dictate the phenomenon, and thirdly solving the governing equations for a specific casting case. In Chapter 2 the phenomena of interest were identified for the basic casting problem. The model used to solve the governing equations will be discussed in the next section.

5.1 Development of the Model

The numerical model in this study will solve the governing equations discussed in Sections 2.4 in a cylindrical coordinate system. The energy equation in two-dimensional cylindrical coordinates becomes:

\[
\rho C_{p,\text{eff}}\left(\frac{\partial T}{\partial t} + v_r \frac{\partial T}{\partial r} + v_z \frac{\partial T}{\partial z}\right) = \frac{1}{r} \frac{\partial}{\partial r}\left(k_r \frac{\partial T}{\partial r}\right) + \frac{\partial}{\partial z}\left(k_z \frac{\partial T}{\partial z}\right)
\]  

(5.1)

The first term in the brackets on the left side of Equation 5.1 represents the transient temperature change, the next two terms in the same bracket are the convective terms associated with liquid material flow. The two terms on the right hand side of Equation 5.1 are the diffusive (conduction) terms which dictate the flow of heat in the solid material. The heat integration method is adopted to account for the latent heat of solidification during the simulation.
The energy equation was initially solved in conjunction with the continuity and momentum equations to obtain an accurate temperature profile in the solidifying melt. In two-dimensional cylindrical coordinates, the continuity, momentum in the r-direction, and momentum in the z-direction equations, respectively, are:

\[
\frac{\partial \rho}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (\rho r v_r) + \frac{\partial}{\partial z} (\rho v_z) = 0
\]

\[
\rho \left( \frac{\partial v_r}{\partial t} + v_r \frac{\partial v_r}{\partial r} + v_z \frac{\partial v_r}{\partial z} \right) = -\frac{\partial P}{\partial r} + \mu_{\text{eff}} \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial v_r}{\partial r} \right) + \frac{\partial^2 v_r}{\partial z^2} \right] - \frac{\mu_{\text{eff}} v_r}{r^2}
\]

\[
\rho \left( \frac{\partial v_z}{\partial t} + v_r \frac{\partial v_z}{\partial r} + v_z \frac{\partial v_z}{\partial z} \right) = -\frac{\partial P}{\partial z}
+ \mu_{\text{eff}} \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial v_z}{\partial r} \right) + \frac{\partial^2 v_z}{\partial z^2} \right] + \rho_{\text{ref}} \beta (T - T_{\text{ref}})
\]

The Boussinesq approximation was used to define the driving force for natural convection, and both a power law scheme, and a graduated material dependent linear function were used to describe the variation of viscosity between solid and liquid control volumes for pure metals and alloys, respectively. The effect of riser shrinkage played no role and was ignored.

5.1.1 DERIVATION OF THE THERMO-MECHANICAL MODEL
The thermo-mechanical model chosen for the study adopted a discretization strategy whereby known continuum mechanics equations were solved for each control volume and additional phenomena were accounted for at each node. The control volume set up is shown in Figure 5.1.

The grid control volumes used to solve the energy equation were chosen as the domain for the thermo-mechanical model. Firstly, a purely elastic, plain-strain description of the cylindrical domain is formulated. From Equations 2.25-2.30, the radial displacement, \( u \), can be expressed for two dimensions in terms of the temperature distribution in the cylindrical casting as:

\[
u = \frac{\alpha}{r(1-\nu)} \left( 1 + v \right) \int_0^r \Delta T \, dr + \frac{(1-3v)R^2}{2} \int_0^R \Delta T \, dr
\]
and in the cylindrical mold as

\[
u = \frac{\alpha}{r(1-v)} \left[ (1+v) \int_r^\infty \Delta T \, dr + \frac{(1-3v)r^2 + R^2(1+v)}{R_m^2 - R^2} \int_r^\infty \Delta T \, dr \right]
\]

(5.6)

Since the temperatures within control volumes are constant, the solution of the temperature integrals can be solved on a piecewise basis, by summing up the volume-weighted terms at every node.

A preliminary modification must be made to these basis elastic equations to make them applicable for two-phase media, since the control volumes in the liquid state are not described by Equation 5.5. During the solidification process, certain control volumes will solidify and can be tracked via the analytical expressions while others are still in their liquid state. When these latter control volumes eventually solidify, in order to maintain the assumption of a material continuum the control volumes have to be assigned an additional thermal potential \( \Delta T \) representative of the cooling that has already occurred in the rest of the solid casting. This thermal potential will increase with time for each new control volume added to the continuum. As an example, assume
CHAPTER 5: NUMERICAL STUDY AND ANALYSIS

an outer ring of the cylinder solidifies and cools to a temperature 100°C below its melting point. Equation 5.5 will estimate the contraction produced by this temperature drop. Next, the center core of the cylinder solidifies, and Equation 5.5 can be applied to its control volumes as it begins to cool from its melting point. From this time forward, Equation 5.5 will record the displacement produced as the center core cools through the complete temperature range from the melting point to room temperature, while during the same time, the outer ring will cool through a temperature range 100°C less. In reality, this will create a thermal mismatch that would have the inner core trying to pull the outer ring towards the center, while the outer core resisted this force. Since the elastic Equation 5.5 is for a continuum, it will not account for this additional potential. The solution around this problem is to introduce an additional temperature potential to the nodes, which solidify later. This can be achieved by raising the apparent temperatures for still liquid nodes, in Equation 5.5, such that each newly solidified node will attempt to cool to a lower temperature than the remaining solid mass, and exert the equivalent contraction potential. The magnitude of this temperature addition is chosen as,

\[
T_{\text{addition}} = \frac{\sum_{\text{nodes=\text{solid}}} (T_{cv} \cdot V_{cv})}{\sum_{\text{nodes=\text{solid}}} V_{cv}} \tag{5.7}
\]

which represents the volumetric mean temperature of the all the solidified nodes to date. The temperature addition is different for each control volume, reflecting the increase in potential as the casting continued to solidify radially inward.

The viscous portion of the model was facilitated via the simplified visco-elastic/plastic strategy developed by Purvis [1] (described in Section 2.4.5) applied to a cylindrical geometry. The accumulated strains at high temperatures were allowed to relax depending on the stress state, temperature and cooling rate of the control volume material. The mechanical properties of the metals and molds can be found in several references [2-5] and Appendix II.

5.1.2 NUMERICAL SOLUTION OF THE GOVERNING EQUATIONS

The governing partial differential equations derived in the previous sections were discretized using a FDM/control volume approach. The equations were solved via the SIMPLER (Semi
Implicit Method for Pressure Linked Equations Revised) algorithm [6]. The SIMPLER algorithm will solve for the energy, continuity, and momentum equations, and any equation, which can be expressed in the following differential form:

\[
\frac{\partial}{\partial t} \left( \rho \phi \right) + \text{div}(\rho \mathbf{u} \phi) = \text{div}(\Gamma \text{grad} \phi) + \text{Source Term}
\]  

(5.8)

where \( \phi \) can be any variable of interest. In our case, the terms in the above equation are defined as:

**ENERGY EQUATION**

\( \phi = T, \Gamma_\phi = k, \text{Source Term} = 0 \) (node accounting methodology is used to account for latent heat via the Heat Integration Method)

**Z-MOMENTUM EQUATION**

\( \phi = v_z, \Gamma_\phi = \mu_{\text{eff}}, \text{Source Term} = -\frac{\partial P}{\partial z} + \rho_{\text{ref}} g \beta (T - T_{\text{ref}}) \) (for constant density)

**R-MOMENTUM EQUATION**

\( \phi = v_r, \Gamma_\phi = \mu_{\text{eff}}, \text{Source Term} = -\frac{\partial P}{\partial r} - \frac{\mu_{\text{eff}} v_r}{r^2} \)

**DISPLACEMENT**

A generic cylindrical displacement model is developed via the theory of thick cylindrical shells for radially varying temperature distributions with thermal relaxation.

The SIMPLER algorithm adopts a TDM solver (the equations are cast into a Tri-Diagonal Matrix and solved via back substitution). A power law scheme is contained within the numerical algorithm to account for the total convective and diffusive flux in the momentum equations. The method adopts a staggered grid approach where temperatures obtained by the energy equation
are evaluated at control volume centers, while velocities from the momentum equation are solved at control volume interfaces. A graphical summary of the model is given below in Figure 5.2.

![Figure 5.2: Overall Model Summary](image)

5.1.3 THE NUMERICAL ALGORITHM
The SIMPLER algorithm has been validated repeatedly in the literature [7][6][8][9][10], and the accuracy of the solution was tested with similar mesh sizes repeatedly in the previous work of the author [11]. The casting model employed in this study has been compared by the author to analytical thermal solutions (the transient radial temperature distribution in an infinite cylinder with an instantaneous change in wall temperature, and the Neumann phase change problem) [7]. Validation has also been performed in comparison with the classic experimental phase change problem conducted by Gau [12] in a gallium filled enclosure. In each case the accuracy of the model was excellent. The interested reader is directed to references [7][11] for more details.
The solution of the governing equations occurs in a semi-coupled fashion, according to the general algorithm shown in Figure 5.4, subject to the boundary conditions outlined Figure 5.3 and Table 5.1.

Equations 5.1-5.4 are solved in a coupled fashion in step 1. The calculation of the thermo-mechanical displacements occurs post iteratively (after the temperature distribution is known) in step 2. Here, Equations 5.5 and 5.6 are solved for solidified nodes, using Equation 5.7 to adjust for thermal inconsistencies (as described in Section 5.1.1), and the relaxation term from Equation 2.51 to include visco-plastic behavior.
### Table 5.1: Boundary Conditions for Thermo-Fluids Model (refer to Figure 5.3)

<table>
<thead>
<tr>
<th>Wall</th>
<th>AB</th>
<th>AC</th>
<th>BD</th>
<th>CD</th>
<th>CE</th>
<th>DF</th>
<th>EF</th>
</tr>
</thead>
<tbody>
<tr>
<td>T</td>
<td>$\frac{\partial T}{\partial r} = 0$</td>
<td>$\frac{\partial T}{\partial z} = 0$</td>
<td>$\frac{\partial T}{\partial z} = 0$</td>
<td>$h = h_{\text{correlated}}$</td>
<td>$\frac{\partial T}{\partial z} = 0$</td>
<td>$\frac{\partial T}{\partial z} = 0$</td>
<td>$T = T_{\text{wall}}$</td>
</tr>
<tr>
<td>$v_r$</td>
<td>$\frac{\partial v_r}{\partial r} = 0$</td>
<td>$\frac{\partial v_r}{\partial z} = 0$</td>
<td>$v_r = 0$</td>
<td>$v_r = 0$</td>
<td>NA</td>
<td>NA</td>
<td>NA</td>
</tr>
<tr>
<td>$v_z$</td>
<td>$\frac{\partial v_z}{\partial r} = 0$</td>
<td>$v_z = 0$</td>
<td>$v_z = 0$</td>
<td>$v_z = 0$</td>
<td>NA</td>
<td>NA</td>
<td>NA</td>
</tr>
<tr>
<td>$u_{\text{metal}}$</td>
<td>$u_{\text{metal}} = 0$</td>
<td>NA</td>
<td>NA</td>
<td>NA</td>
<td>NA</td>
<td>NA</td>
<td>NA</td>
</tr>
<tr>
<td>$u_{\text{mold}}$</td>
<td>NA</td>
<td>NA</td>
<td>NA</td>
<td>NA</td>
<td>NA</td>
<td>NA</td>
<td>NA</td>
</tr>
</tbody>
</table>

---

Solve for the energy equation and any other pertinent equations (Navier-Stokes, mass transfer, etc.) for a given time step

Numerically calculate the thermal contraction and determine the air gap size

Use the correlation to determine the local heat transfer coefficient

Modify the boundary at the mold/metal interface for the next iteration

Repeat until cooling is complete

---

Figure 5.4: Numerical Solution Algorithm
Using the correlations developed in Chapter 4, the heat transfer coefficients are calculated after every iteration, based on the predicted size of the air gap in step 3. Finally, in step 4, the boundary conditions for the equations solved in step 1 are updated, and the procedure repeats forward in time until the desired interval is reached. The results of the numerical model for each system studied are given in the next section.

5.2 Numerical Results

A numerical trial was run for each of the experiments in Table 3.3. The numerical prediction of the air gap size as a function of time will be shown relative to the experimental real time measurements for comparison. As discussed in Section 3.3.4, the experimental gap measurements were assumed to approximate radial symmetry within about 8-12%.

Several trials revealed that the contribution of the continuity and momentum equations to the overall change in displacement at the metal surface was negligible. This is shown in Figure 5.5

![Figure 5.5 The Negligible Effect of Accounting for Flow in the Melt on the Prediction of Gap Size](image)
for the pure aluminum-copper system, which experiences the greatest natural convection flow (the plot will be fully described in a subsequent section, and is presented here only to illustrate the simplification).

Thus, the complexity of the model could be reduced, and only the energy equation was solved, without any appreciable loss of accuracy. This result was expected from earlier modeling work in casting systems. The thermo-mechanical component of the model will be validated in the next section via comparison to experimental measurements.

5.2.1 PURE ALUMINUM-GRAPHITE MOLD SIMULATIONS
The air gap prediction plot for pure aluminum cast in a graphite mold is given in Figure 5.6, which depicts three curves.

![Figure 5.6: Numerical Air Gap Predictions for the Pure Aluminum-Graphite System](image)

Two numerical results are shown: the visco-elastic/plastic model, and a purely elastic model to illustrate the effect of high temperature relaxation. The visco-elastic/plastic model shows a
smaller air gap for a given time interval than the purely elastic model. This difference is caused by the inability of the softer hot material to contract towards the geometric center of the casting as efficiently as when the material is assumed to be purely elastic.

Note that both numerical models appear to lag the experimental measurements at the outset. This lag is probably due to the phase change algorithm employed in the thermal model, which causes a slight inflection point during the solidification of the metal. The inflection disappears when the model is run for alloys, where solidification occurs over a temperature range, and the temperature profile near the interface is more accurate.

A complete discussion of the inaccuracies associated with temperature measurements at the solid-liquid interface generated by various phase change algorithms was given by Salcudean and Abdullah [13]. Nevertheless, both solutions effectively approximate both the magnitude and the rate of air gap formation satisfactorily.

![Figure 5.7: Numerical Air Gap Predictions for the A356-Graphite System](image)

- experimental data
- numerical, elastic, correlated htc
- numerical, visco-elastic/plastic, correlated htc
5.2.2 A356-GRAPHITE MOLD SIMULATIONS
Similar plots for the A356-graphite system are given in Figure 5.7. The smaller overall thermal contraction associated with A356 contributes to a larger relative error in the prediction of the total displacement. The high temperature viscous effects are more pronounced as solidification now occurs over a temperature range, and the difference between the pure elastic and visco-elastic/plastic curves is larger. Here, the elastic curve overestimates the contraction at all times, while the visco-elastic/plastic curve initially is late in predicting the moment of formation, and later slightly over predicts the experimental data.

5.2.3 TIN-GRAPHITE MOLD SIMULATIONS
The tin-graphite system contained the greatest amount of experimental error. Thus it was anticipated that the model would possibly not agree very closely with the experimentally recorded air gap formation data. In Figure 5.8, both the numerical elastic and visco-elastic/plastic curves overestimated the overall size of the gap by a considerable amount relative to the minimal contraction observed.

![Figure 5.8: Numerical Air Gap Predictions for the Tin-Graphite System](image)
CHAPTER 5: NUMERICAL STUDY AND ANALYSIS

These results were expected, since the tin-graphite system exhibited a minute amount of contraction as illustrated in Chapter 3. Still the system was analyzed to test the capability of the LVDTs in conditions that required the utmost precision. In general, the air gap data was sound, with the exception of the plateau in the gap size at later times, despite the expected uncertainty with the LVDT. The only area where more reasonable agreement was achieved was in the prediction of the approximate start time of the gap, which is more a reflection of the accuracy of the thermal model used in this study.

5.2.4 PURE ALUMINUM-COPPER MOLD SIMULATIONS
The numerical air gap plots in copper molds differed significantly from the graphite mold simulations. The rapid cooling rate of the copper molds generally resulted in a steeper air gap formation curve and higher stress levels in the solidifying casting. Nowhere was this more evident than in the pure aluminum-copper system trials (Figure 5.9).

![Graph of air gap size vs. time for pure aluminum-copper system](image)

Figure 5.9: Numerical Air Gap Predictions for the Pure Aluminum-Copper System
The air gap formation plot for pure aluminum is seen to increase rapidly within 50 seconds to a high value (over 0.2 mm) and subsequently slows to a lower rate as phase change is completed and the air gap approaches its final size. The difference between the elastic and visco-elastic/plastic model curves occurs early in the formation process, and remains relatively constant after about 75 seconds.

5.2.5 A356-COPPER MOLD SIMULATIONS
When A356, was cast into the copper mold the numerical simulation (Figure 5.10) predicted the slower air gap formation associated with A356, and the difference between the two numerical models occurred almost immediately. Both models resulted in good agreement for all recorded times.

Figure 5.10: Numerical Air Gap Predictions for the A356-Copper System

5.2.6 A206-COPPER MOLD SIMULATIONS
The A206-copper system and the Al-4wt%Cu-copper systems represented castings with the widest mushy ranges, and hence the difference between the pure elastic and visco-elastic/plastic...
models in these systems was the greatest. The air gap formation plot for A206 was very similar in nature to the A356 plot with the exception of the drastic difference between the two numerical models. This difference was also documented in the work of Vicente-Hernandez [14]. For these systems, the use of a purely elastic model may introduce error that is of an equivalent or even higher magnitude than the experimental error, and hence an elastic heat transfer coefficient-air gap correlation will not perform as well for wide mushy range alloys. The relative difference between the numerical curves in Figure 5.11 substantiates this observation in comparison to the difference in Figure 5.10.

![Graph showing air gap prediction models](image)

**Figure 5.11: Numerical Air Gap Predictions for the A206-Copper System**

### 5.2.7 Al-4wt%Cu-Copper Mold Simulations

Since the thermophysical properties for Al-4wt%Cu and A206 did not differ appreciably, the numerical output plots for both of these cases (Figures 5.11-5.12) are identical. The only difference between the plots is in how the experimental curves for the air gap relate to the numerical output. The same visco-elastic/plastic model shows good agreement with both the
A206 and Al-4wt% Cu experimental curves, indicating that both the numerical and experimental techniques are sound. The next section will explore how this agreement between numerical and experimental results can be used to extrapolate a correlation in cases where an experimental correlation cannot be formulated conventionally.

5.3 Numerical Applications

The primary numerical application for a model of this type has already been explored in the previous section, where the model was used to more accurately predict the formation of the gap, which is a measure of the instantaneous mold cooling rates. A less obvious application is to use the model as a developmental tool for formulating approximate correlations where experiment techniques prove inefficient. The typical sand mold offers such a case.
5.3.1 SAND CASTING APPLICATIONS
When casting in sand molds, the difficulty in measuring the formation of the air gap experimentally was soon realized. The LVTD connecting rods could not be adequately fastened to the mold inner wall, and local changes in sand structure made thermal contraction measurements unreliable. Thus, the air gap could not be experimentally measured with any creditability, and the formation of a correlation was not possible. However, since the heat transfer coefficient can still be measured with a good degree of accuracy, the model could run using the experimentally measured values of heat transfer coefficient as a function of time to predict the thermal contraction of the casting. Once a numerical curve of the air gap formation is produced (see Figure 5.13), the data can be used in conjunction with the experimental heat transfer coefficient curve to generate an approximate experimental/numerical correlation. This correlation will prove useful if a variation on the casting process is introduced which causes a change, for example, in the rate of formation of the air gap. In this case, the correlation could still

![Figure 5.13: Experimental Heat Transfer Coefficient and Numerical Air Gap Predictions for Pure Aluminum Cast in a Sand Mold](image-url)
provide boundary condition values, where the previous heat transfer coefficient values (used prior to the variation) would prove inadequate.

A sand casting experiment was conducted to implement the aforementioned strategy, and obtain a working correlation for aluminum castings. The experiment remained the same as was described in Chapter 3, and as expected, the LVDT data measured was meaningless. Only the heat transfer coefficient could be estimated from thermocouple data for this experiment. Using a curve fit, the heat transfer coefficient was input to the model as a function of time, and the real time output of air gap size was predicted. A plot of the predicted air gap and the measured heat transfer coefficient is given in Figure 5.13. From this plot, the inverse correlation equation developed in Chapter 4 could be applied. The regression analysis for the aluminum-sand system is shown in Figure 5.14.

![Figure 5.14: Correlation Plot for Commercial Purity Aluminum Cast in a Sand Mold](image)

Correlation Coefficient = 0.9875

- $r = 8.05 \times 10^{-3}$
- $k = 0.171$
- $C = 1.84$
The heat transfer coefficient for sand molds is considerably less than any system examined to date, yet the curves were seen to closely fit the inverse correlation equation. Care must be taken in applying this correlation indiscriminately, however, since no validation for the air gap formation was possible as was with correlations developed in Chapter 4. The use of the model for these types of applications should be accompanied with several trials to insure the repeatability of the results.

5.4 Model Improvements Facilitated by the Technique

The main goal behind the development of our correlation strategy was to improve the performance of a given casting simulation model. If this goal is not met, then the overall value of the work becomes academic at best. In this section, the difference in the accuracy of the model facilitated by coupling thermal boundary conditions with the formation of the air gap is investigated. This difference will be shown to be significant for each of the various casting cases examined in this study.

A typical numerical model run without boundary condition coupling will be compared with an identical model where the boundary conditions have been coupled using the correlations in this study. The ‘non-coupled’ model will be run under a best-case scenario, where the selection of the constant heat transfer coefficient value will be made such that the final predicted air gap size is nearly identical to the experimentally measured size. This is achieved by running successive numerical trials, and adjusting the value of the input heat transfer coefficient until the air gap sizes match up precisely. Although in practice, this technique is not possible, it represents the upper limit that can be achieved using a constant heat transfer coefficient model. If the coupled model can improve upon this limit, then its inclusion in the numerical scheme is definitely worthwhile. The difference in performance for the experimental systems in this study will convince the reader of the need for boundary condition coupling in estimating cooling rate dependent phenomena such as microstructure prediction and hot tearing estimation.
5.4.1 Pure Aluminum-Graphite Mold Simulation Improvement

The aluminum-graphite system will initially be used to illustrate the magnitude of the difference between models incorporating constant and variable heat transfer coefficients. Figure 5.15 depicts four numerical curves and an experimental curve for comparison.

![Graph showing numerical and experimental data comparison](image)

**Figure 5.15: Comparison between Conventional and Coupled Models for the Aluminum-Graphite System**

Two of the numerical curves represent the variable correlated heat transfer coefficient models shown previously in Section 5.2. The remaining two curves were generated using a 'best case' constant heat transfer coefficient. Although the constant heat transfer coefficient can be chosen such that the air gap formation after a given time interval is comparable, the path and rate of formation of the gap will contain severe deficiencies. In this case, the air gap does not begin to form until about 100 seconds after the experimentally observed curve. Its magnitude does not begin to increase significantly until about 180 seconds, at which point the experimental curve has already reached almost 90% of its final value. This slowness in response is typical for casting
simulations (with the exception of continuous casting), since the heat transfer coefficient will always decrease with time. Thus, the use of a constant heat transfer coefficient will necessarily introduce a lag into the predicted response from the mathematical model. This lag will reoccur in differing degrees for each system considered in this work.

5.4.2 A356-GRAPHITE MOLD SIMULATION IMPROVEMENT
Figure 5.16 gives the equivalent curves for the A356-graphite system. The difference between the constant and variable heat transfer coefficient models for A356 was less pronounced than in the pure aluminum-graphite system. In Figure 5.16, if one considers all four models together, the lag exhibited by the constant heat transfer coefficient models appears to be no more significant than the error exhibited by the elastic-variable heat transfer coefficient model. Focusing solely on the visco-elastic/plastic models, however, the difference becomes much more significant.

---

**Figure 5.16: Comparison Between Conventional and Coupled Models for the A356-Graphite System**
The smaller gap magnitudes in this system tend to further reduce the degree of lag exhibited, as compared to the pure aluminum casting.

5.4.3 Tin-Graphite Mold Simulation Improvement
As noted previously, the experimental study with tin anticipated a large degree of scatter with respect to the LVDT readings. The thermal model of tin being cast, however, experienced no such difficulties, and the lag exhibited in the previous systems was also detectable with tin. The curves in Figure 5.17 reveal that the correlated heat transfer coefficient models performed much better, especially at the start of the air gap formation. The copper molds revealed a similar trend, and will be examined in the next section.

![Figure 5.17: Comparison Between Conventional and Coupled Models for the Tin-Graphite System](image)

5.4.4 Pure Aluminum-Copper Mold Simulation Improvement
The greatest discrepancies between the numerical models were seen in the pure aluminum-copper system. Figure 5.18 illustrates the extent of the difference, and the three experimental results
confirm the deficiencies of the uncoupled model. Any cooling rate predictions made on the basis of the constant heat transfer coefficient model would severely undershoot the initial high degree of cooling, and subsequently, badly overshoot the cooling rate near the end of the process. To

![Graph showing air gap size over time for different models.](image)

**Figure 5.18: Comparison Between Conventional and Coupled Models for the Aluminum-Copper System**

date, this problem will exist in many commercial packages used in industry, that can accurately predict the overall solidification times and average temperature gradients, but often fail in the prediction of hot tearing during the solidification of larger castings.

### 5.4.5 A356-COPPER MOLD SIMULATION IMPROVEMENT

The constant and variable heat transfer coefficient models for the A356-copper system appear in Figure 5.19. The constant heat transfer coefficient model performed a little better in this system, and showed less lag than average. This improvement was primarily due to the fact that the extremes between maximum and minimum heat transfer coefficients were lower for A356, and
the constant heat transfer coefficient model has less ground to ‘catch up’. The performance of the visco-elastic/plastic correlated heat transfer coefficient model was still far superior.

5.4.6 A206-COPPER MOLD/AL4wt%CU-COPPER MOLD SIMULATION IMPROVEMENT

The trend in A356 was also evident with A206. Again the differences between the elastic and the visco-elastic/plastic models make it difficult to distinguish the extent of the lag error, but focusing on the visco-elastic/plastic model clarifies this deficiency. The Al-4wt%Cu casting behaved essentially in the same manner as in Figure 5.20.
Figure 5.20: Comparison Between Conventional and Coupled Models for the A206/Al-4wt%Cu-Copper System
Chapter References


Summary and Conclusions

A summation of the findings of this study are presented and discussed.

The diverse nature of this project allowed for an exploration of many casting phenomena, and the conclusions presented in this section are equally diverse, ranging from experimental observations to efficiency improving numerical strategies. The conclusions are presented alongside a chapter by chapter summary, reflecting some of the more essential details of each section as appropriate.

7.1 Conclusions

The first chapter represented the problem identification stage of the study, where the main reasons for carrying out the work were presented. The scope of the endeavor was outlined with the hope of overcoming some elementary shortcomings with the typical casting simulation. Although able to predict the overall average cooling rate, current numerical casting models may suffer from an inability to accurately predict changes in cooling rate if accurate time-varying boundary conditions are not specified. As a result, constant heat transfer coefficient models would be unable to predict cooling rate dependent phenomena such as final microstructure and hot tearing.

This deficiency led to an investigation to determine the most influential factor responsible for inducing a change in the cooling rate of a casting. The formation of an air gap at the metal-mold interface was isolated as the most significant variable, and a systematic approach (not limited to a specific industrial process) was undertaken to quantify the heat transfer coefficient-air gap relationship across a varying range of molds with varying thermophysical properties and surface
roughness. A numerical strategy was formulated which required the development of a deformation model. Unfortunately this requirement lead to the discovery that the complex rheology of metals near their melting point has resulted in discrepancies in accounting for their thermo-mechanical behavior. Hence, the formulation of the thermo-mechanical model involved an investigation into current ultra-high temperature material behavior theory. Much disagreement was observed in these literature studies. Nevertheless, with the help of some basic assumptions, a reasonable existing model was adopted, and found to be acceptable for our casting set up.

In Chapter 3, the experimental work necessary for implementing the boundary condition coupling strategy was described:

I. Heat transfer coefficients and air gap sizes could be more accurately measured using experimental techniques designed and optimized in this study.

For the majority of metal-mold systems, the experimental set up gave acceptable results, though the data was still seen to contain quantifiable errors, which became moderately problematic for low contraction castings. Error analysis was used to confirm the reliability of the experimental results, and identify significant limitations.

The expected inverse relationship between the wall heat transfer coefficient and the air gap was observed for all metal-mold systems. Also noted was the intense reduction in the overall heat flux out of the casting with the initial formation of the air gap, an important consideration for mold designers.

In Chapter 4, the functional form of the inverse relationship was proposed:

II. A semi-empirical inverse equation of the form \( htc = \frac{1}{k \cdot A + r} + C \) was found to best characterize the relationship between the heat transfer coefficient and air gap for all metal-mold systems considered.
CHAPTER 6: SUMMARY AND CONCLUSIONS

This equation accounted for the uncertainty present when the surface roughness asperities are of similar magnitude to the air gap size. Previous comparable documented studies had relied on at least three different straight-line segments, fit from data obtained by means of a process specific experimental set up.

The general heat transfer coefficient equation was also applied to data from the literature:

III. The proposed form of inverse function was able to accurately describe the relationship between heat transfer coefficient and air gap for data documented in the literature.

The inverse equation fit the reported data very well, although only a limited amount of data points were reported. The constants of the inverse equation varied considerably between the experimental trials of this study and the literature, and among similar trials in the literature, due to undocumented experimental variables in many published works. These variables were responsible for significant effects on Stage II and III heat transfer coefficients (see Section 2.5.1).

In the numerical work presented in Chapter 5, the proposed thermomechanical model was formulated and was shown to give acceptable results:

IV. A simplified visco-elastic/plastic model was developed for a cylindrical coordinate system to estimate the air gap formation during casting. The model's predictions were accurate in comparison with the experimental measurements.

The model was introduced into a casting simulation and, by incorporating the derived correlations into the numerical scheme of the previously 'best case' constant boundary condition model, the coupling strategy became fully implemented. The effect of the coupling strategy on the predicted air gap formation was examined at various times during casting.

V. The implemented coupling strategy improved the accuracy of the uncoupled heat transfer coefficient casting model, eliminating the associated time lag and bettering the predicted air gap formation rates.
For this reason, only a coupled model could expect to function reasonably during the early stages of the casting process. The choice of model was seen to be less important than the actual coupling component present:

**VI. The purely elastic model consistently overestimates the air gap formation by a small amount, though for practical purposes, a correlation based on an elastic model will generally give acceptable results.**

The simplified visco-elastic/plastic model does, however, appear to be the better choice for more general applications.

An interesting application of the model was its use in remedying, at least roughly, the inability to form a correlation with the absence of key LVDT data, during casting in sand molds:

**VII. The numerical model can be used to generate a correlation in the absence of complete experimental measurements.**

Although not recommended for completely new systems, the strategy can be effective when minor casting changes are implemented.

In Chapter 4, the complete set of experimental results from the preceding chapters were converted into a non-dimensional form. The most influential observation involved the transient nature of the surface roughness effect on the heat transfer coefficient. The surface roughness greatly reduced the effective heat transfer coefficient, at least an order of magnitude lower than predicted by the analytical expression, for perfectly flat surfaces, in every system examined for very small gap sizes.

**VIII. The effect of roughness on the overall heat transfer coefficient was greatest for small gap sizes, during the initial formation and growth of the gap, and dropped off as the gap size increased.**

At larger gap sizes, the effect of roughness becomes negligible, and the measured heat transfer coefficient approached the analytical value predicted for a perfectly flat surface.
CHAPTER 6: SUMMARY AND CONCLUSIONS

7.2 Future Work

Often a study of this type will generate more questions than it answers. Although full closure was obviously not possible, subsequent studies in this field can be directed into additional valuable endeavors. This project will conclude with a list of possible research topics, designed to address inquiries left unexplored.

- Additional experimental trials designed to produce specific microstructures or hot tearing can be compared with both coupled and non-coupled models to observe any improvement.

- Equivalent coupled models can be developed for coated molds, and during process changes in water-cooled continuous casting (where the operating parameters are suddenly modified producing non steady state conditions).

- Dimensional analysis with secondary variables not explored in this study on the heat transfer coefficient could be performed. These studies would vary the following parameters: the properties of the gas in the gap (i.e., cast in a helium environment), the size of the casting and the geometry of the interface for large gap formations. Additionally the mold metal interfacial roughness could be examined comprehensively for a given mold material. This could result in a more general non-dimensional analysis.

- An analytical model for thermomechanical mushy state behavior can be developed and validated.
Appendix I
CALCULATION OF RELATIVE LVDT ERROR
APPENDIX I

THE FOLLOWING DERIVATION OUTLINES LVDT ERROR ASSOCIATED WITH THE THERMAL EXPANSION OF THE CONNECTING RODS

The temperature variation between the LVDT connecting rods is very minimal in our casting trials for the following reasons. The position of the two rods differs by at most 3 mm, with the metal LVDT extending into the mold and the mold LVDT being flush with the mold inner surface. The remaining lengths of both rods are subjected to identical boundary conditions through the length of the mold wall. Hence, as we move towards the mold interior, when the temperature of the metal LVDT rod drops to the temperature of the mold LVDT rod, any additional expansion will be experienced identically by both rods and will introduce no relative error. Thus, we need only estimate how much of the metal LVDT rod is at a higher temperature than the mold LVDT and calculate the maximum expansion possible.

If we assume that the temperature distribution in the LVDT connecting rods can be approximated by fin theory*, then the temperature distribution is given by:

\[
\frac{T - T_m}{T_o - T_m} = \frac{\cosh[m(L - x)]}{\cosh[mL]} = e^{-m(x)} \text{ for an infinite fin (when } m > 2.65) \]

where \( m = \sqrt{\frac{hP}{kA_c}} \).

\( h \) is the heat transfer coefficient between the fin and the mold, \( P \) is the fin perimeter, \( k \) is the fin thermal conductivity, and \( A_c \) is the cross sectional area of the fin.

Substituting the worst case values of \( h = 100 \text{W/m}^2/\text{°C}, P = 2\pi(0.00125), k=40 \text{W/m}^2/\text{°C}, \) and \( A_c = \pi(0.00125)^2 \) \((0.001055)^2\) yields a value of \( m = 120.1 \). With \( T = 460^\circ\text{C}, T_m = 20^\circ\text{C} \) and \( T_o = 660^\circ\text{C} \) (the maximum temperature of the mold fin), solving the above equation for \( x \) results in a value of 3.12 mm.

The total magnitude of the error is thus

\[
\text{error} = \Delta l = \alpha \Delta TL
\]

where \( \Delta l \) is the total expansion error, \( \alpha \) is the coefficient of thermal expansion equal to 0.000016 1/°C, \( \Delta T \) is the maximum temperature difference across the mold-metal interface equal to 200°C, and \( L \) is the value for \( x \) (3.12 mm) calculated above. The solution to this equation with the above parameters yields a value for the error of 0.00998 mm.


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Appendix II

THERMOPHYSICAL PROPERTIES OF VARIOUS MEDIA, compiled from references [1-15]
## APPENDIX II

### Commercial Purity Aluminum [average properties are at 723 K]

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### A356 Aluminum Alloy (6.5-7.5wt% Si, 0.6wt% Fe, 0.25wt% Cu, 0.35wt% Mn, 0.2-0.45wt% Mg, 0.35wt% Zn, 0.25wt% Ti) [average properties are at 723 K]

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A206 Aluminum Alloy (0.1wt% Si, 0.1wt% Fe, 4.2-5.0wt% Cu, 0.2-0.5wt% Mn, 0.15-0.35wt% Mg, 0.05wt% Ni, 0.1wt% Zn, 0.05wt% Sn, 0.15-0.3wt% Ti) [average properties are at 723 K]

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Al-4wt%Cu Aluminum Alloy [average properties are at 723 K]

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### Physical Properties

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<td>232 °C</td>
</tr>
<tr>
<td>Emmissivity</td>
<td>0.06</td>
</tr>
<tr>
<td>Density</td>
<td>7300 kg/m³</td>
</tr>
</tbody>
</table>

### Copper Mold [average properties are at 723 K]

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal Conductivity</td>
<td>377 W/m/K</td>
</tr>
<tr>
<td>Specific Heat Capacity</td>
<td>385 J/kg/K</td>
</tr>
</tbody>
</table>

### Mechanical Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Poisson's Ratio</td>
<td>0.3</td>
</tr>
<tr>
<td>Coefficient of Thermal Expansion</td>
<td>1.77 × 10⁻⁶ K⁻¹</td>
</tr>
</tbody>
</table>

### Physical Properties

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Emmissivity</td>
<td>0.64</td>
</tr>
<tr>
<td>Density</td>
<td>8940 kg/m³</td>
</tr>
</tbody>
</table>
**APPENDIX II**

Graphite Mold [average properties are at 723 K]

<table>
<thead>
<tr>
<th>Thermal Properties</th>
<th>solid</th>
<th>liquid</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal Conductivity</td>
<td>15 W/mK</td>
<td></td>
</tr>
<tr>
<td>Specific Heat Capacity</td>
<td>1000 J/kgK</td>
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</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Mechanical Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Poisson's Ratio</td>
</tr>
<tr>
<td>Coefficient of Thermal Expansion</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Physical Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Emissivity</td>
</tr>
<tr>
<td>Density</td>
</tr>
</tbody>
</table>

Sand Mold [average properties are at 723 K]

<table>
<thead>
<tr>
<th>Thermal Properties</th>
<th>solid</th>
<th>liquid</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal Conductivity</td>
<td>0.94 W/mK</td>
<td></td>
</tr>
<tr>
<td>Specific Heat Capacity</td>
<td>800 J/kgK</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Mechanical Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Poisson's Ratio</td>
</tr>
<tr>
<td>Coefficient of Thermal Expansion</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Physical Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Emissivity</td>
</tr>
<tr>
<td>Density</td>
</tr>
</tbody>
</table>

**Thermal Conductivity of Graphite as a Function of Temperature**

\[ k_{\text{graphite}} = 1.8 \times 10^{-5} \, T(\degree C)^2 - 2.6 \times 10^{-2} \, T(\degree C) + 19.38 \]
Figure A2.1: Thermal Conductivity of Air as a Function of Temperature

Figure A2.2: Thermal Conductivity of Copper as a Function of Temperature
Figure A2.3: Thermal Conductivity of Green Sand as a Function of Temperature

Appendix References


Appendix III

EXPERIMENTAL ERROR BAR PLOTS
Figure A3.1: Maximum Heat Transfer Coefficient and Air Gap Size Error in an Aluminum-Graphite System

Figure A3.2: Maximum Experimental Error in an Aluminum-Graphite System Correlation
Figure A3.3: Maximum Heat Transfer Coefficient and Air Gap Size Error in an A356-Graphite System

Figure A3.4: Maximum Experimental Error in an A356-Graphite System Correlation
Figure A3.6: Maximum Experimental Error in a Tin-Graphite System Combination

Heat Transfer Coefficient (W/m²K)

Air Gap Size (mm)

Time (seconds)

Heat Transfer Coefficient (W/m²K)
Figure A3.7: Maximum Heat Transfer Coefficient and Air Gap Size Error in an Aluminum-Copper System, Trial I

Figure A3.8: Maximum Experimental Error in an Aluminum-Copper System Correlation, Trial I
Figure A3.9: Maximum Heat Transfer Coefficient and Air Gap Size Error in an Aluminum-Copper System, Trial II

Figure A3.10: Maximum Experimental Error in an Aluminum-Copper System Correlation, Trial II
Figure A3.11: Maximum Heat Transfer Coefficient and Air Gap Size Error in an Aluminum-Copper System, Trial III

Figure A3.12: Maximum Experimental Error in an Aluminum-Copper System Correlation, Trial III
Figure A3.13: Maximum Heat Transfer Coefficient and Air Gap Size Error in an A356-Copper System

Figure A3.14: Maximum Experimental Error in an A356-Copper System Correlation
Figure A3.15: Maximum Heat Transfer Coefficient and Air Gap Size Error in an A206-Copper System

Figure A3.16: Maximum Experimental Error in an A206-Copper System Correlation
Appendix IV

RESIDUAL PLOTS FROM THE REGRESSION ANALYSIS OF ALL CORRELATED SYSTEMS
Figure A4.1: Plot of Residual Errors for the Aluminum-Graphite System

Figure A4.2: Plot of Residual Errors for the A356-Graphite System
Figure A4.4: Plot of Residual Errors for the Aluminum-Copper System

Figure A4.3: Plot of Residual Errors for the Tin-Copper System
Residual Error for Equation $1/(a+b^x)+c$

Figure A4.5: Plot of Residual Errors for the A356-Copper System

Residual Error for Equation $1/(a+b^x)+c$

Figure A4.6: Plot of Residual Errors for the A206-Copper System
Figure A4.7: Plot of Residual Errors for the Al-4wt%Cu-Copper System
IMAGE EVALUATION
TEST TARGET (QA-3)

1.0  1.4  1.6
1.25
1.1  1.8
1.25  1.4  1.6

150mm

6″

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