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Assessment of the Accuracy of a Computational Casting Model

by

Robertus Tjin Hok Tjoa

B.A.Sc.Eng., University of Ottawa, Ottawa, Canada, 1989

**A thesis submitted to the Faculty of Graduate Studies
and Research in partial fulfilment of the requirements for
the degree of**

Master of Engineering

**Department of Mechanical and Aerospace Engineering
Ottawa-Carleton Institute for Mechanical and Aeronautical Engineering
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submitted by
Robertus Tjin Hok Tjoa
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the degree of Master of Engineering

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Abstract

The investigation in this thesis concerns the numerical prediction of the solidification of castings. Two aspects are treated: the first is the measurement of the thermal properties of molding sands, and the second addresses the issue of whether accurate predictions can be made with the present solidification algorithms. Accurate computer predictions of the solidification of castings are only possible provided that accurate input data is available; these include the geometry, the boundary conditions, the initial conditions, and the material properties. It is important to know the thermal properties of the molding sand accurately as these strongly influence the rate of heat extraction from the casting and thereby the quality of the casting produced.

Due to the wide variety of molding sands available, it is often necessary to conduct extensive laboratory examinations to determine the temperature dependent thermal properties of these sands. This process would be greatly facilitated if accurate in-situ methods for the determination of these properties were available. An examination of such methods is conducted in the first part of this thesis. It is found that while several approaches have been proposed, an accurate method of this nature does not exist.

Extensive validation of a solidification code developed at Carleton University was conducted in the second part of this thesis. The results from four validation tests are reported. The first test is analytical. The remaining three compare numerical predictions with measured results from, respectively, an Al-7Si casting, a ductile iron casting, and an induction furnace steel casting. The predictions from these tests show good overall agreement with the experimental results.

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versteckt im Hintergrund
die ganze Zeit war'n Sie
Wörter die ich brauchte
vergessen werd' ich nie ...

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List of Symbols

C	capacitance matrix
C_l	liquidus composition
C_o	bulk alloy composition
C_p	specific heat per unit mass
c_p	specific heat per unit volume $c_p = \rho C_p$
C_s	solidus composition
C_E	carbon equivalent
f_g	fraction of grain
f_i	internal fraction of solid
f_s	fraction of solid
FEA	finite element analysis
FEM	finite element method
h	heat transfer coefficient
H	enthalpy
k	thermal conductivity
K	stiffness matrix
L	latent heat of fusion
$\dot{n}$	nucleation rate
Q	heat source
r	radial coordinate
R, R_g	radius of grain
S	thickness of solidified casting
t	time
T	temperature

T_i	initial temperature condition
T_{int}	casting/mold interface temperature
T_M	melting point of cast metal
T_o	step imposed temperature at a boundary
$T(x, t, \alpha)$	computed temperature at location x , time t for an estimated α
$\tilde{T}(x, t)$	measured temperature at location x , time t
v	advance velocity of solid/liquid interface
x	cartesian coordinate
α	thermal diffusivity
α'	computed estimate for α
α_E	finite difference computed thermal diffusivity
$\delta\alpha_m$	error on computed thermal diffusivity due to measurement
$\delta\alpha_t$	error on computed thermal diffusivity due to truncation
Δt	chronological spacing
ΔT	temperature difference or undercooling
Δx	positional spacing
Ω	supersaturation
ρ	density
θ	integration scheme parameter
Θ	normalized temperature

Chapter 1

Overview

The purpose of any computer simulation is to provide accurate predictions of the physical processes being modelled. In the area of casting, the goal is the accurate prediction of thermal histories and solidification patterns. To make accurate predictions one must have accurate data and use fully validated software. Data such as geometry, boundary and initial conditions, and material properties must be known; this may be particularly difficult for the mold. Mold properties which govern the cooling rate of castings may vary considerably. Current research efforts attempt to categorize sands and archive the available data into data bases [1, 2] or devise simple methods of thermal property measurement [3, 4, 5, 6, 7].

Closed form solutions for typical casting shapes do not exist. Except for the simplest of cases, where analytical solutions are available, numerical solutions must be employed. As computing power becomes cheaper and more accessible, numerical methods will become a common tool in casting design. Prior to extensive use, however, comparison of computed predictions with analytical and experimental results will be required to demonstrate the validity of any software.

The principal objective of this thesis was to establish a methodology for evaluating the accuracy of a computational analysis of the solidification of castings. Two issues were involved. First, could an inexpensive, reliable method for in-situ determination of thermal properties be devised; a method appropriate for use on the foundry floor? Second, given the uncertainty in the values of material properties, could accurate predictions be made with current solidification algorithms? It quickly

becomes clear how inseparable these issues are. Both will be reviewed in this thesis.

This main body of this thesis is divided into two broad parts: The first part, contained in chapter 2, addresses the issue of thermal property determination. The second part, encompassing chapters 3 and 4 examines the issue of software validation.

1.1 Introduction on thermal property determination

The thermal history and solidification pattern indicates the heat transfer characteristics from the casting. This plays a major role in determining the quality of the casting produced. The rate of heat extraction is strongly influenced by the thermal properties of the mold. Accurate knowledge of these properties is therefore essential in developing reliable computer simulations. While the thermal properties of typical cast iron, steel, and aluminum alloys are fairly well known, those of molding sands are not. Owing to the wide variety of sand mixtures, existing data bases for their properties are limited. The thermal properties of sands are a function of sand composition, water content, compacting method, hardness, hardness uniformity and, in particular, temperature [1, 2, 4, 5]. For this reason, data regarding the temperature dependence of molding sand thermal properties, particularly thermal conductivities show wide scatter [8].

Many researchers have examined methods for determining these properties. An in-situ method for property determination would be preferred over laboratory type methods. The advantages are obvious. When obtained under conditions similar to the actual application, such as those of a foundry floor as opposed to a laboratory, much more confidence can be placed on the results. Methods applied on the foundry floor are less likely to result in preparational differences in the sand; as mentioned before thermal properties are influenced greatly by many factors such as composition and density to name a few. Batch-to-batch variations in the sand will be detected

more easily using tests done on the foundry floor. In-situ methods would of course be much more economical as well since no special equipment or floor conversions would be required.

While much research has been done on thermal property determination, most methods are not suitable for the foundry floor or fail to accurately predict temperature dependence. Possibly the most promising method, albeit of a laboratory nature, was proposed by O. Krischer [6]. This was a quasi steady state method which permitted simultaneous measurement of the temperature dependent thermal conductivity, specific heat and thermal diffusivity. It was especially suited for measurement of specific heat of poorly conducting solids and for samples of high moisture content. Parallel plates of test material of equal thickness were interleaved with heater filaments. A constant heat flux from the heaters would produce parabolic quasi-stationary temperature fields across the plates. This allows computation of temperatures and gradients as a function of time, and hence thermal properties directly.

P. Kannaiah *et al* [4] employed a Casting-Over Probe Embedded Specimen Method. This method measures temperature with thermocouples embedded in a circular plug which forms the central part of the base of a cylindrical mold. The thermocouples monitor temperatures at varying distances from the casting/mold interface at the base. The thermal diffusivity is eventually computed from an empirical relationship. This method does not, however, produce temperature dependent property values. A more recent technique proposed by Luo *et al* [7] used temperature measurements for the one-dimensional heat flow from a flat rectangular pure copper casting. The resulting thermal history and temperature profile upon complete solidification were then approximated by first order parabolic equations; these were used to obtain three separate expressions of the quantity of heat released by the casting and absorbed by the mold. Their simultaneous solution would yield apparent thermal property values. While Luo's method is suitable for use in foundry

workshops, it only computes apparent thermal property values and does not account for temperature dependence.

In part I of this thesis three in-situ methods are discussed. The first two, proposed by M.J. Kirt and E. Schürman, were taken from published literature. An additional method, employing a least square minimization approach, was also examined.

M.J. Kirt *et al* [5] applied a finite difference approach to the axisymmetric heat equation. While this was a lab experiment, the same approach could be adapted to the foundry floor. In the experiment a sand cylinder with thermocouples embedded at mid-height was heated in a resistance-heated tube furnace. Temperature as a function of radius at specified times was approximated by fitting an even power series summation to the experimental data by least square regression. This together with an assumed linear development of temperature with time allowed a finite difference solution for the thermal diffusivity.

E. Schürman [3] proposed a simple scheme to compute the temperature dependent thermal diffusivity based on one-dimensional heat flow in a semi-infinite solid body. The thermal diffusivity is directly extracted from the normalized heating curves of several thermocouples. This approach appeared very promising as it is an in-situ method and is relatively easy to apply.

A method examined by the author involves the approach of assessing the accuracy of the thermal diffusivity due to a finite difference approach by studying the behaviour of the sum of the squares of temperature differences. This approach will subsequently be referred to as the *Least Square Method*. Such a method is robust and well established for data fitting analyses. For the present application it has the additional advantage of being completely independent of the casting geometry or dimensionality. The method basically minimizes the error between measured temperatures and temperature fields computed by successive choices of diffusivity values. Actual thermal properties should coincide with the minimum error in the

resulting curves.

1.2 Introduction on software validation

The second part of this thesis discusses the issue of validation of an FEM-based casting software developed at Carleton. This is an integral part of the software development. Validation tests involve the comparison of numerical predictions with experimental measurements or analytical solutions. In the present application thermal histories and solidification patterns are commonly compared. The sequence of the tests conducted demonstrates the validity of the software on two levels. The first level validates the mathematical basis of the software; this is done by comparing the computed results with analytical solutions. The second, and more important level, demonstrates the applicability of the software to real physical cases; this is done by comparing the numerical predictions with experimental results. This second level is also the more difficult of the two.

Three solidification models were used for the validation tests; they will be called the first and second latent heat models and the Rappaz model. The first latent heat model is a very basic model which does not consider the microstructural evolution during solidification. This model assumes a solid fraction of zero above the melting point in the case of pure metals (or the liquidus temperature in the case of eutectic alloys) and a solid fraction of one below the solidus temperature (or the eutectic temperature in the case of eutectic alloys). Essentially a well defined planar solidification front is assumed, where the temperature at the liquid/solid interface remains constant until all the latent heat has been released.

The second latent heat model [9] is more complete in that it provides some prediction of the mushy zone characteristic of non-eutectic alloys. During solidification, at temperatures between the liquidus and solidus, the fraction of solid as a function of undercooling is computed by employing the lever rule for equilibrium conditions.

While this is only an approximation of the actual solid formation, tests indicate that the results do not differ much from more comprehensive models such as that of Rappaz. This latent heat model, of course, also has the advantage of being very simple; only a few well known material parameters are needed. During cooling from the liquidus to the solidus temperature only five parameters are needed: the liquidus and solidus temperatures, the latent heat of fusion, the specific heat, and the fraction of solid at the solidus temperature. These are easily obtained.

The final model, proposed by M. Rappaz [10, 11, 12], deals with the solidification of equiaxed microstructures. While equiaxed dendritic solidification is frequently encountered in casting, it is more difficult to model. The growth of new grains is now related to local undercooling; the formation of dendrites, diffusion of solute and heat have to be taken into account simultaneously. Rappaz's model is more comprehensive in accounting for the growth kinetics of the grains, the thermal balance and the solute balance including the diffusion of solute outside the dendritic grain. While the model is more comprehensive the large number of input parameters, most of which are not well known for most alloys, make it more difficult to use.

Of the tests conducted, four are reported in this thesis. The first validates the software against an analytical solution; the first latent heat model is used in this case. The last three tests compare the software predictions with experimental results taken from published literature. The first of these experimental validations, compares results from an aluminum alloy casting [13]. The Rappaz model was used for this test since the input parameters are well known for this case. The second experiment is a cylindrical ductile iron casting [14]; here the first latent heat model was used. The last case is an induction furnace steel casting [15]. Due to the large solidification range reported for this last experiment, the second latent heat model was used.

Chapter 2

Thermal Property Determination

Solidification of alloys is primarily controlled by heat diffusion and to some extent by convection within the liquid region. In the absence of convective effects, the basic equation governing solidification expresses the conservation of energy as:

$$\text{div}(k\nabla T) = c_p \frac{dT}{dt} - L \frac{df_s}{dt} \quad (2.1)$$

with:

k	thermal conductivity – $W/(m \ K)$
T	temperature – K
c_p	volumetric specific heat – $J/(m^3 \ K)$
t	time – <i>sec</i>
L	volumetric latent heat of fusion – J/m^3
f_s	fraction of solid

In the case of simple heat conduction without solidification ($df_s/dt = 0$) , i.e. the condition in the mold and in all solidified portions of the casting, the latent heat term does not appear. Treatment of the latent heat evolution during solidification is complicated and is managed by either the latent heat models or the Rappaz model mentioned earlier. In this thesis repeated reference will be made to the case of one-dimensional heat flow. For this case equation 2.1 becomes:

$$\frac{\partial}{\partial x}(k \frac{\partial T}{\partial x}) = c_p \frac{dT}{dt} - L \frac{df_s}{dt}$$

where x indicates the position in one dimension.

All the methods for the property determination examined here make use of a standard solution for one-dimensional transient flow which can be found in any fundamental heat transfer text [16]. The description follows. A semi-infinite solid extends from $x=0$ to $x=\infty$ and has an initial temperature T_i . The temperature at its surface, $x=0$, is suddenly changed to and maintained at T_o . The thermal properties of the solid, here expressed by the thermal diffusivity α , are constant. The analytical solution for the temperature distribution in the solid is:

$$T(x, t) = T_o + (T_i - T_o) \operatorname{erf}\left(\frac{x}{2\sqrt{\alpha t}}\right) \quad (2.2)$$

This distribution, in turn, can be used to compute the heat flow at any x position in the solid as a function of time, t . The Gauss error function is defined as:

$$\operatorname{erf}\left(\frac{x}{2\sqrt{\alpha t}}\right) = \frac{2}{\sqrt{\pi}} \int_0^{\frac{x}{2\sqrt{\alpha t}}} e^{-\eta^2} d\eta$$

Figure 2.1 is a schematic of the problem.

Three methods will be discussed in the following sections. They are: (1) a finite difference approach proposed by Kirt *et al* [5], (2) a method by Schürman *et al* [3], and (3) the accuracy assessment by the sum of squares. The first two are taken from published literature, while the last method is examined by the author. These methods compute the thermal diffusivity. There appears to be a greater scatter among data reported for thermal conductivities than there is for specific heat. As such, the specific heat of molding sands is more readily available. As well, when unknown, the specific heat is not very difficult to measure and could be found easily by standardized laboratory methods.

Figure 2.1: Diagram of the analytical conduction problem

The examinations are generally conducted in two stages. First, the methods are applied to a case of constant thermal diffusivity to show that the method works. Since such conditions are simple, these tests are expected to yield correct results. In the second stage, the methods are tested for the more difficult situation involving temperature dependent properties. This is accomplished by generating simulated experimental data by numerical means, such as FEM, and applying the proposed method to these results.

2.1 Finite Difference Property Determination

M.J. Kirt *et al* [5] examined a finite difference method to compute the temperature dependent thermal diffusivity and conductivity for a dry molding sand. Previous research on thermal properties indicated that the specific heat of molding sands is reasonably well known as a function of temperature. If thermal diffusivities can be accurately obtained, then thermal conductivities can be computed from the ratio of the diffusivity to the specific heat.

The finite difference method suggested by Kirt allows the measurement of temperature dependent thermal diffusivity. This method was conceived as an in-lab experimental procedure. Although it was not intended as an in-situ test, it could

potentially be adapted for use in a foundry workshop. In Kirt's experiment a hollow copper cylinder with thermocouples embedded at mid-height was filled with sand, hand-rammed, and furnace dried to a given hardness. The cylinder was long enough to ensure essentially one-dimensional heat flow at the thermocouple plane; this was verified experimentally by two redundant thermocouples. The cylinder was then placed in a resistance heated vertical tube furnace and heated from 27°C (80°F) to 816°C (1500°F). Measurements were taken by the thermocouples to determine the variation of temperature as a function of radial position and time. The temperature dependent thermal diffusivity was computed from this data. The thermal conductivity could be found by using published data for the density and specific heat.

The heat equation in cylindrical coordinates appears as follows:

$$\rho C_p r \frac{\partial T}{\partial t} = \frac{\partial}{\partial r} \left(k r \frac{\partial T}{\partial r} \right)$$

This equation can be rewritten as (refer to Appendix B for details):

$$\alpha(T_i) = \frac{\frac{\partial T}{\partial t}|_{t_i, r_i} - \frac{1}{\rho C_p} \frac{\partial k}{\partial T}|_{T_i} \left(\frac{\partial T}{\partial r} \right)^2|_{t_i, r_i}}{\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right)|_{t_i, r_i}} \quad (2.3)$$

with:

ρ	density - kg/m^3
C_p	specific heat - $\text{J}/(\text{kg } ^{\circ}\text{C})$
r	radial position - m
T	temperature - $^{\circ}\text{C}$
t	time - sec
k	thermal conductivity - $\text{W}/(\text{m } ^{\circ}\text{C})$

The second part of the numerator in equation 2.3 was neglected by Kirt *et al.* It was shown that the error caused by this omission, at no more than 1%, was smaller

than the 2% to 3% error found in experimental data. This omission was therefore justified.

Equation 2.3 can be solved if the variation of temperature with position and time could be established. At each time step a polynomial relating temperature to radial position was obtained by applying least square regression to the thermocouple readings. With the resulting functional relationship of temperature to position, the denominator of equation 2.3 could easily be computed. Furthermore, if the temperature was assumed to vary linearly with time during the small time interval (Δt) between successive thermocouple readings, a simple forward difference expression for the numerator could be found: $\frac{\partial T}{\partial t}|_{t_i, r_i} = \frac{T(r_i)_{t_i + \Delta t} - T(r_i)_{t_i}}{\Delta t}$. The temperature dependent thermal diffusivity is found very simply with the above procedure.

Various sources of error could arise in such a method. The polynomial approximation for the temperature in itself magnifies any measurement errors which may have occurred. As well, any finite difference relationship has inherent errors due to the truncation of higher order terms. Such a method may not be practical if the accumulated errors overwhelm the accuracy of the results.

2.1.1 Finite difference error analysis

For the present examination, the basic method proposed by Kirt *et al* was modified slightly. The modifications allowed the use of a real casting and mold in place of the furnace and cylindrical plug of mold sand. 1-D heat flow was assumed to exist in the mold. The thermal diffusivity was computed from the temperature histories measured by thermocouples placed in the mold. The resulting finite difference method is very similar to that of Kirt *et al*.

The practicality of the finite difference approach for the determination of the thermal diffusivity was assessed. The examination was performed for two mold types: a sand mold, which extracts heat slowly, and a cast iron mold, which is es-

entially a chill. An error analysis was performed to determine if an in-situ type method could be employed on a small casting with reasonable confidence. Since some approximation of typical experimental data is necessary this examination was conducted with conditions for which an analytical solution exists. The one-dimensional heat flow case described earlier will be used here; the heated surface at $x=0$ can be likened to the casting/mold interface. Temperature independent thermal properties are involved in this case.

The one-dimensional heat equation is easily rearranged to yield the thermal diffusivity as:

$$\alpha = \frac{\partial T}{\partial t} / \frac{\partial^2 T}{\partial x^2} \quad (2.4)$$

A slight change from Kirt's approach is used by applying the finite difference discretization to the denominator as well as the numerator of equation 2.4. The finite difference expression becomes:

$$\alpha_E = \frac{\Delta T_2}{\Delta t} / \frac{T_1 - 2T_2 + T_3}{\Delta x^2} \quad (2.5)$$

with:

T_1, T_2, T_3	temperatures at nodes 1, 2 and 3 respectively - °C
ΔT_2	$(T_2^{n+1} - T_2^n) - °C$
Δx	spacing between thermocouples - m
Δt	time increment - sec
n	current increment
$n + 1$	subsequent increment

The central difference expression for $\partial^2 T / \partial x^2$ requires the use of three thermocouples. To reduce the number of design parameters the thermocouples are spaced equally a distance of Δx apart. The first thermocouple is located at a distance x_1

from the casting/mold interface. The computation of α_E requires measurement of three temperatures T_1 , T_2 and T_3 at time t and a further measurement of T_2 at time $t + \Delta t$. Four design parameters now exist: t , Δt , x_1 and Δx .

Equation 2.2, with a diffusivity α , would be used to generate the experimental temperatures for the desired design parameters. Substitution of these results into equation 2.5 would enable a study of the behaviour and magnitude of these resulting errors.

The purpose of this section was to examine the behaviour and magnitude of the relative errors in the computed diffusivity, α_E , for various combinations of the above design parameters. This should provide an indication of the feasibility of this method. There are two contributors to the error in the computed diffusivity, $\delta\alpha$:

1. A truncation error contribution, which will be denoted $\delta\alpha_t$, is due to the truncation of higher order terms in the finite difference expression. Equation 2.5 assumes a constant heating rate $\partial T/\partial t$ and a uniform curvature in the temperature distribution $\partial^2 T/\partial x^2$.
2. A measurement error due to the instrumentation limits with regard to measurement of temperature, time, and location. The respective instrument limits are: δT , δt and δx . Errors of this nature are grouped as $\delta\alpha_m$. In this investigation the basic instrumentation errors were taken as: $\delta x = \pm 0.0005 \text{ m}$ and $\delta t = \pm 0.5 \text{ seconds}$. Two different values for δT were looked at: $\pm 5^\circ\text{C}$ and $\pm 0.25^\circ\text{C}$.

The truncation error, $\delta\alpha_t$, is easily computed from the difference between the finite difference computed diffusivity, α_E (see equation 2.5), and the actual diffusivity, α , used in the analytical solution (see equation 2.2). If the measurement errors δT , δt and δx were zero, the finite difference computed diffusivity would still differ from the actual diffusivity solely due to the truncation errors.

$$\delta\alpha_t = \frac{\alpha - \alpha_E}{\alpha_E} \quad (2.6)$$

Here α_E represents the value computed by equation 2.5. This expression is limited in accuracy by the assumption of a constant heating rate $\partial T/\partial t$ and a constant curvature in the temperature distribution $\partial^2 T/\partial x^2$. Since the thermal diffusivity, α , used in the analytical solution is known, the difference between the two values is due to the finite difference discretization. The relative error due to this truncation is then as expressed in equation 2.6.

The assessment of the measurement error, α_m , is somewhat more complicated. The independent variables are: T_1 , T_2 , T_3 , ΔT_2 , Δt and Δx , i.e. the diffusivity will be regarded as the following function:

$$\alpha = \alpha(T_1, T_2, T_3, \Delta T_2, \Delta t, \Delta x)$$

The errors due to the differences in temperature, time and location: $\delta \Delta T_2$, $\delta \Delta t$, and $\delta \Delta x$ result from the basic instrumentation errors as follows:

$$\begin{aligned}\delta \Delta T_2 &= \sqrt{(\delta T_2^n)^2 + (\delta T_2^{n+1})^2} \\ \delta \Delta t &= \sqrt{2(\delta t)^2} \\ \delta \Delta x &= \sqrt{2(\delta x)^2}\end{aligned}$$

The absolute error can be found by taking the total derivative of equation 2.5:

$$\begin{aligned}d\alpha &= -\frac{\Delta T_2 \Delta x^2 \delta T_1}{\Delta t (T_1 - 2T_2 + T_3)^2} + \frac{2 \Delta T_2 \Delta x^2 \delta T_2}{\Delta t (T_1 - 2T_2 + T_3)^2} \\ &\quad - \frac{\Delta T_2 \Delta x^2 \delta T_3}{\Delta t (T_1 - 2T_2 + T_3)^2} + \frac{\Delta x^2 \delta \Delta T_2}{\Delta t (T_1 - 2T_2 + T_3)} \\ &\quad - \frac{\Delta T_2 \Delta x^2 \delta \Delta t}{\Delta t^2 (T_1 - 2T_2 + T_3)} + \frac{2 \Delta T_2 \Delta x \delta \Delta x}{\Delta t (T_1 - 2T_2 + T_3)}\end{aligned}\tag{2.7}$$

Dividing the above equation by equation 2.5 results in a relative error expression:

$$\begin{aligned}
\delta\alpha_m = & -\frac{\delta T_1}{T_1 - 2T_2^n + T_3} + \frac{2\delta T_2^n}{T_1 - 2T_2^n + T_3} \\
& -\frac{\delta T_3}{T_1 - 2T_2^n + T_3} + \frac{\delta\Delta T_2^n}{\Delta T_2^n} \\
& -\frac{\delta\Delta t}{\Delta t} + \frac{2\delta\Delta x}{\Delta x}
\end{aligned} \tag{2.8}$$

Since the sign of any individual error is not known, an RMS summation of these terms is preferred. Such a summation of the terms comprising $\delta\alpha_m$ and $\delta\alpha_t$ will result in a complete expression for the relative error in the thermal diffusivity computed by equation 2.5:

$$\delta\alpha = \sqrt{\sum_i \delta_i^2} \quad i = 1, 2, \dots, 7 \tag{2.9}$$

where the terms δ_i indicate the term contributions from $\delta\alpha_t$ and $\delta\alpha_m$; i.e. the single term from equation 2.6 and the six terms comprising equation 2.8.

The behaviour of this error is now examined by varying the four design parameters: t , Δt , x_1 and Δx . The best set of parameters balances the error contributions in such a manner as to minimize the overall error, $\delta\alpha$. The difficulty here, of course, is that while certain changes may decrease some contributions, they may increase others. The simplest way to examine this behaviour is to select an acceptable range for all four parameters and to calculate the error for all combinations at various intervals. Alternatively for specific values of any two parameters it is possible to search for the remaining two parameters yielding the lowest error, $\delta\alpha$. Results from this latter approach produces a series of surface plots fixed for two parameters with the other two as independent variables. Since these results are easier to interpret, this approach was used. In the present study locations and times were taken as

Figure 2.2: Error sensitivity to time

pairs; for example if $(x, \Delta x)$ is specified then the search is conducted for $(t, \Delta t)$, and vice versa. As with any search over discrete values, however, the difficulty remains in that any solution is limited by the size of the search step. Figure 2.2 is a sample surface plot where the pair of $(x, \Delta x)$ is specified; figure 2.3 is a similar plot for the case where $(t, \Delta t)$ is specified. From these curves, the behavioural trend of the relative error $\delta\alpha$ is easily seen. The minimum occurs over a narrow region, with errors quickly exceeding acceptable levels. It is also of interest to note that the placement of the first thermocouple need not necessarily be very near or at the casting/mold interface.

While the present investigation compared results to an analytical solution which involved constant thermal properties, the mechanism for a temperature dependent

Figure 2.3: Error sensitivity to thermocouple location

case would essentially remain the same. An additional term similar to the one shown in equation 2.3 would appear. The contribution of this additional term for the complete differential equation was small for the casting case examined by Kirt. In any case, this term cannot be computed beforehand as it requires knowledge of the temperature dependent thermal conductivity and was therefore omitted in the present investigation as well.

The test conditions for both types of mold were kept the same with a constant pouring temperature, $T_o = 650^\circ C$, and an initial temperature of the mold, $T_i = 350^\circ C$. This pouring temperature and the range between the pouring and initial temperatures are low for sand mold applications. However, maintaining identical conditions would serve to provide a basis of comparison.

Results for the cast iron mold indicate that this finite difference approach is not particularly practical. Table 2.1 below shows some of the results obtained for the

$x_1 \rightarrow$ $\Delta x \downarrow$	0.000 (m)	0.001 (m)	0.002 (m)	0.005 (m)	0.010 (m)
0.010	34 (2, 4)	34 (2, 4)	31 (2, 8)	25 (3, 12)	23 (7, 16)
0.015	21 (5, 8)	21 (6, 8)	21 (6, 8)	17 (4, 20)	15 (9, 28)
0.020	15 (9, 12)	15 (10, 12)	15 (13, 16)	13 (5, 28)	11 (11, 40)
0.025	12 (17, 20)	12 (18, 20)	12 (18, 20)	12 (5, 48)	9 (13, 56)

Table 2.1: Cast Iron mold: minimum possible error on α_E with $\delta T = \pm 0.25^\circ\text{C}$. $(t, \Delta t)$ as indicated in brackets.

cast iron mold; the temperature accuracy for this case was $\delta T = \pm 0.25^\circ\text{C}$. While typical thermocouple errors are larger than this, the results of using such optimistic values serve to demonstrate the difficulty in obtaining accurate thermal property measurements. The thermal diffusivity for the cast iron mold was taken as $\alpha = 5.85 \times 10^{-6} \text{m}^2/\text{s}$. This table was produced by specifying the locational pair $(x, \Delta x)$ as indicated in the column and row headers respectively. Within the table are listed the minimum relative error (as a percentage) along with the corresponding t and Δt pair shown in brackets. The time, t , was searched in 1 second intervals while the time step, Δt , was searched in 4 second intervals. The results are therefore limited by this step size. Chill molds are usually on the order of 0.05 m thick. The table indicates that, for practical values of $(x, \Delta x)$, expected relative errors are roughly 10% or greater. Such values are barely acceptable. Errors less than this could only be achieved for much greater mold sizes or unreasonably long experimental time periods.

$t \rightarrow$ $\Delta t \downarrow$	50 (sec)	200 (sec)	500 (sec)	1000 (sec)	5000 (sec)
50	26 (0.000, 0.010)	32 (0.000, 0.023)	45 (0.023, 0.015)	65 (0.030, 0.020)	∞
200	20 (0.005, 0.015)	13 (0.000, 0.023)	14 (0.000, 0.033)	18 (0.000, 0.048)	43 (0.008, 0.093)
500	17 (0.005, 0.028)	11 (0.010, 0.025)	8 (0.000, 0.033)	9 (0.000, 0.048)	18 (0.010, 0.090)
1000	15 (0.003, 0.028)	9 (0.008, 0.030)	8 (0.015, 0.033)	6 (0.000, 0.045)	9 (0.005, 0.098)
5000	11 (0.003, 0.063)	7 (0.008, 0.080)	5 (0.013, 0.078)	4 (0.018, 0.070)	3 (0.000, 0.100)

Table 2.2: Sand Mold: minimum possible error on α_E with $\delta T = \pm 0.25^\circ C$. $(x, \Delta x)$ as indicated in brackets.

A similar examination was conducted for a sand mold. The thermal diffusivity used in the analytical solution for the sand mold was $\alpha = 2.78 \times 10^{-7} m^2/s$. Results from these tests indicate that it may be possible to employ the finite difference approach if extreme care is taken in controlling experimental errors. Only results for the $\delta T = \pm 0.25^\circ C$ error are quoted here. If the measurement error δT is as much as $\pm 5^\circ C$ the relative errors $\delta\alpha$ are much larger and the method becomes impractical. Thermocouple measurement errors are expected to lie between these limits. Table 2.2 displays the results when $(t, \Delta t)$ is fixed as indicated in the row and column headers. The table entries are the percent relative error $\delta\alpha$ with the corresponding $(x, \Delta x)$ pair in brackets beneath it. The third row of this table indicates that it is possible to achieve relative errors less than 10% for mold dimensions of about 10 cm; for example, for $(t, \Delta t) = (500, 500)$ seconds a relative error of 8% was found at $(x, \Delta x) = (0.000, 0.033)$ m. Such dimensions are still reasonable for sand molds. Table 2.3 shows the results in similar format for specified values of $(x, \Delta x)$.

$x_1 - \Delta x \downarrow$	0.000 (m)	0.001 (m)	0.002 (m)	0.005 (m)	0.010 (m)
0.010	24 (50, 80)	24 (50, 80)	23 (60, 90)	21 (60, 220)	20 (130, 420)
0.015	16 (110, 150)	17 (120, 160)	17 (140, 170)	15 (80, 400)	13 (200, 490)
0.020	13 (200, 250)	13 (220, 260)	13 (240, 270)	12 (100, 610)	11 (270, 620)
0.025	10 (320, 270)	10 (350, 380)	11 (370, 390)	11 (450, 430)	10 (470, 570)

Table 2.3: Sand Mold: minimum possible error on α_E with $\delta T = \pm 0.25^\circ C$. $(x, \Delta x)$ as indicated in brackets.

The bracketed values within the table now indicate the corresponding $(t, \Delta t)$ pair produced by the search for the minimum $\delta \alpha$. Practical locational values for $(x, \Delta x)$ would be approximately $(0.005, 0.05)$ m. Table 2.3 indicates that reasonable errors can be achieved even at dimensions much smaller than these. It would suggest that this method may be of use for molds with low thermal diffusivities such as sand.

Any experiment conducted on the basis of this method would have to be performed with great diligence. It is important to note that it is not possible to obtain the temperature dependent thermal diffusivity accurately for a fixed triad of thermocouples. Table 2.3 indicates when to take the temperature readings at a particular set of thermocouples. This implies that readings taken at times different than those indicated for the specified $(x, \Delta x)$ would produce greater errors in the computed diffusivity. To apply the finite difference method with great accuracy one would first have to construct complete tables similar to those shown. Temperature measurements to be used in a finite difference expression such as equation 2.5 would have to

be made at the times and locations indicated by these tables. Measurements made elsewhere would carry larger, possibly unacceptable, errors.

2.1.2 Kirt's method re-examined

A closer examination of the method proposed by Kirt *et al* was conducted to confirm the conclusions drawn thus far with regard to the finite difference approach. This examination was conducted by numerically simulating the experimental procedure outlined by Kirt *et al* in their paper [5]. Similar geometry and thermocouple locations were used.

The gradual heating of a cylindrical sand mass with known thermal properties was simulated numerically. The temperature of its outer surface was raised from 20°C to 1000°C linearly with time. Only axisymmetric heat conduction was involved. The cylindrical mass had a radius of 0.0381 m (1.5 in.) with thermocouples located at every $6.35 \times 10^{-3}\text{ m}$ (0.25 in.) from the central axis. This resulted in six thermocouple locations at which temperatures were monitored.

The equation used for this analysis is the finite difference equation 2.3. As suggested by Kirt *et al*, some terms in the numerator were neglected to yield:

$$\alpha(T_i) = \frac{\frac{\partial T}{\partial t}|_{t_i, r_i}}{\frac{1}{r} \frac{\partial}{\partial r} (r \frac{\partial T}{\partial r})|_{t_i, r_i}} \quad (2.10)$$

with

r radial position - m
 T temperature - $^{\circ}\text{C}$
 t time - sec

With a polynomial curve fitted to the measured temperature and radial position and the assumption of a linear variation of temperature with time in each time step, the thermal diffusivity can easily be computed.

The time intervals, Δt , for the numerical simulation were selected between 2.5 and 25.0 seconds during the early stages. At later times, especially for the longer running simulations, even larger time increments were permissible as the linear assumption in the thermal histories became increasingly more accurate. The cycle time in Kirt's actual experiment was 16 seconds.

At the selected time intervals the temperatures at the six thermocouples were fitted to polynomials of degree n . From these polynomials, the denominator of equation 2.10 was computed at each thermocouple location. The thermal diffusivity was associated with the temperature at each location at the present time. A relationship between the thermal diffusivity and temperature was then obtained.

In addition to any experimental measurement errors, several other factors can affect the accuracy of the results:

1. The heating rate of the outer surface of the cylinder.
2. The degree of polynomial curve fitted at each time step.
3. The spacing between the thermocouples (Δx).
4. The size of the time increment (Δt).

Of these factors, the last two were found to have minimal effect on the results. Halving the thermocouple spacing had minimal effect on the scatter of the computed diffusivities; at the same time, the resulting spacings of roughly 0.003 m would be difficult to achieve experimentally. Increasing the time increment also had minimal effect on the results. In fact the computed curves for the larger time steps, while less dense due to the decreased sampling times, were coincident with their counterparts over most of the temperature range. Slight differences in the computed diffusivity curves were noted at low temperatures (well below 100°C) because the linear assumption in the heating rate is not highly accurate during this period.

The largest influence on the accuracy of the computed diffusivity is exerted by the heating rate and the degree of polynomial curve-fit. Three cases will be discussed in this regard. They are outlined as follows:

- TEST case I

Overall duration of experiment :	2500 <i>sec</i> (0.7 <i>hrs</i>)
Heating rate of outer surface :	0.392°C/ <i>s</i>
Degree of polynomial :	2 (figure 2.4)
	6 (figure 2.5)

- TEST case II

Overall duration of experiment :	10000 <i>sec</i> (2.8 <i>hrs</i>)
Heating rate of outer surface :	0.089°C/ <i>s</i>
Degree of polynomial :	2 (figure 2.6)
	10 (figure 2.7)

- TEST case III

Overall duration of experiment :	36000 <i>sec</i> (10.0 <i>hrs</i>)
Heating rate of outer surface :	0.0272°C/ <i>s</i>
Degree of polynomial :	2 (figure 2.8)
	10 (figure 2.9)

This method is very sensitive to both position and degree of polynomial fit for the temperature-position function when high heating rates are involved. Figure 2.4 clearly shows the separation in the computed diffusivity curves due to positional differences. Large positive errors are exhibited by locations nearest the outer surface of the cylinder, the most rapidly heated region. While the higher degree of polynomial for the case of figure 2.5 improves the lower temperature results, it raises the errors

Figure 2.4: Comparison of actual thermal diffusivity and those computed at various thermocouple positions. Heating rate: 0.392°C/s ; Degree of polynomial : 2

Figure 2.5: Comparison of actual thermal diffusivity and those computed at various thermocouple positions. Heating rate: 0.392°C/s ; Degree of polynomial : 6

Figure 2.6: Comparison of actual thermal diffusivity and those computed at various thermocouple positions. Heating rate: 0.089°C/s ; Degree of polynomial : 2

Figure 2.7: Comparison of actual thermal diffusivity and those computed at various thermocouple positions. Heating rate: 0.089°C/s ; Degree of polynomial : 10

Figure 2.8: Comparison of actual thermal diffusivity and those computed at various thermocouple positions. Heating rate: 0.0278°C/s ; Degree of polynomial : 2

Figure 2.9: Comparison of actual thermal diffusivity and those computed at various thermocouple positions. Heating rate: 0.0278°C/s ; Degree of polynomial : 10

in the higher temperature range to roughly 25% relative error at its highest point. This increase in error and scatter toward the higher temperatures with increased degree of curve-fit is seen in all the test cases.

The second test case revealed that reasonably accurate results can be obtained with lower heating rates. The results for the lower temperature range were improved markedly with the higher degree of polynomial (figure 2.7). While errors in the higher temperature range became more biased when the degree of polynomial was increased, the relative error remained below approximately 8% at worst.

The final case shows that for very slow heating rates, i.e. prohibitively long experiment durations, very accurate results can be obtained through most of the temperature range with only a second degree polynomial. In fact, the scatter about the actual diffusivity curve and the error became markedly worse when a higher degree was used.

These results are consistent with the finite difference error analysis of section 2.1.1. The trend followed by the progression from case 1 (high heating rate) to case 3 (low heating rate) indicate that rapid heating of one surface causes the finite difference method to be excessively sensitive to thermocouple positioning. Errors due to position may, as a result, become very large. For cases involving high heating rates, errors only decrease late into the experiment, after the thermal gradients have become less severe. This is clearly exhibited in figure 2.4 by the better agreement of the computed thermal diffusivity at higher temperatures. It is therefore not feasible to employ a finite difference approach in a strictly in-situ method for the purpose of determining the thermal properties.

While the finite difference method proposed by Kirt *et al* can be made to produce fairly accurate results (for example figure 2.8), there remains a difficulty in choosing a proper heating rate and degree of curve-fit. In addition, several hours of experimental and computing time would be necessary to obtain these results. Another difficulty with the extended duration of the necessary experiments is that

time dependent influences due to the effects of the binders, entrapped gases, or water vapour in green sands would not be properly reflected in the results.

2.2 Schürman's method

E. Schürman [3] proposed an in-situ method for the determination of the temperature dependent thermal diffusivity. His experiment was based on the error function solution, described earlier, for one-dimensional flow in a semi-infinite body. Schürman noted that equation 2.2 can be rewritten in a dimensionless form, as a normalized temperature:

$$\Theta = \frac{T_o - T}{T_o - T_i} = \operatorname{erf}\left(\frac{x}{2\sqrt{\alpha t}}\right) \quad (2.11)$$

This equation dictates that graphs of temperature (normalized, Θ , or actual, T) when plotted against $x/(2\sqrt{\alpha t})$ or $x/(2\sqrt{t})$ must fall on a single line. With temperatures measured experimentally, these curves can easily be extrapolated to the surface, $x=0$, to determine the surface temperature ($T_{x=0}$).

Several tests using cast iron (%C varying from 3.3% to 4.58%) in a quartz sand mold (99.6% SiO_2) were conducted. Due to their volume to surface area ratio, one dimensional flow can be most readily assumed for flat plates. Schürman studied $0.150 \times 0.150 \times 0.018$ m rectangular ingots of cast iron. The mold was sufficiently thick to ensure that no heat escaped to the outside until solidification was complete. The pouring temperature lay between 1370°C and 1400°C while the initial temperature of the mold was 20°C . Two thermocouples were placed in the casting; one in the center and one at the interface. Four thermocouples were placed in the mold at 0.002, 0.0077, 0.017, 0.0303 m from the casting/mold interface.

Schürman's method begins with the determination of the contact temperature (temperature at the casting/mold interface). This was accomplished in several ways. The simplest came from the measurements taken by the interface thermocouple; this

Figure 2.10: Schürman's experimental curve for normalized temperatures: I. Θ vs. $\frac{x}{2\sqrt{t}}$; II. $\text{erf}(\frac{x}{2\sqrt{\alpha t}})$

was determined at $1070 \pm 20^\circ \text{C}$. He also determined this temperature by extrapolating the curve for T vs. $x/(2\sqrt{t})$ to the interface surface; this resulted in $1070 \pm 10^\circ \text{C}$. At the end of the experiment, the resulting thermal property values were used to compute the interface temperature again, by a separate formula; the result confirmed the previous values.

Figure 2.10 shows two curves plotted against the same abscissa; both represent the same temperature field. The first curve, I, shows the experimental Θ vs. $x/(2\sqrt{t})$. The second curve, II, represents equation 2.11; this is really the error function where the independent variable represents $x/(2\sqrt{\alpha t})$. For the same ordinate value, the ratio of the two abscissa is $1/\sqrt{\alpha}$. The thermal diffusivity at the temperature indicated by the ordinate (Θ) is then easily obtained by dividing the two corresponding abscissa values. According to Schürman repeating this for several different temperatures will produce the temperature dependence of the thermal diffusivity.

2.2.1 Constant (Analytical) α case

To first test our understanding of Schürman's method, an examination was conducted on the simplest case. The analytical case for the one-dimensional transient heat flow in a semi-infinite body was used. Conditions were chosen to match Schürman's experiment as closely as possible. A thermal diffusivity (α) of $5.556 \times 10^{-7} \text{ m}^2/\text{s}$ was used. The initial temperature (T_i) was set at 20°C and the imposed boundary temperature (T_o) was taken as 1070°C . As in the actual experiment, temperatures were computed at five locations: 0, 0.002, 0.0077, 0.017, and 0.0303 m .

Figure 2.11 depicts the thermal history of the five nodes for roughly the same time span as Schürman's experiment. Figure 2.12 shows the single curve obtained for T vs. $x/(2\sqrt{t})$; also, the intersection at the surface $x=0 \text{ m}$ indicates the contact temperature at 1070°C as expected. Figure 2.13 is the normalized temperature curve from which the diffusivity is eventually computed. The resulting diffusivity curve, determined by Schürman's method, is shown in figure 2.14. We can conclude from this that the method works, at least for constant thermal property cases.

2.2.2 Temperature dependent α case

The more significant case is the determination of temperature dependent properties. To examine this, a simple one dimensional conduction problem was considered once again. This time experimental temperatures were simulated numerically by FEM calculations to generate thermal histories for a known temperature dependent diffusivity. Schürman's method when applied to these histories should be capable of returning the original property used in the simulation. A semi-infinite body was used; the far end being insulated. The semi-infinite condition is satisfied so long as the insulated end has not yet experienced a temperature change. A 1 m long mesh was used to ensure this. The mesh is shown in figure 2.15.

Figure 2.11: Thermal histories from analytical test case

Figure 2.12: Thermal history as a function of $\frac{x}{2\sqrt{t}}$ from analytical test case

Figure 2.13: Curve I: Normalized Temperature and Curve II: Gauss Error Function; from analytical test case

Figure 2.14: Computed thermal diffusivity from analytical test case

Figure 2.15: FEM mesh used for temperature dependent α test

Figure 2.16: FEM computed thermal history at five node locations for temperature dependent α case

Figure 2.17: Curve I: FEM computed normalized temperature and Curve II: Gauss Error Function; for temperature dependent α case

Figure 2.18: Comparison of thermal diffusivities; Curve I: FEM input, curve II: output from Schürman's method

Five thermal histories were extracted to simulate the experimental measurements obtained by Schürman. The temperature dependent diffusivity used as input to the finite element analysis is shown as curve II in figure 2.18. These properties are typical of silica sands. The initial temperature of the mold was taken at 20°C . A temperature of 1070°C was imposed at the casting/mold interface ($x=0\text{ m}$) at time $t=0\text{ sec}$.

The resulting thermal histories are shown in figure 2.16. Curves 1 to 5 represent Schürman's five thermocouple locations. The normalized temperature curve (corresponding to figure 2.10) is shown as curve I in figure 2.17; curve II on the same figure represents the error function, $\text{erf}[x/2(\sqrt{\alpha t})]$. Following the prescribed method, the two abscissa values corresponding to a series of ordinate values were divided to compute the thermal diffusivity, α . For example (refer to figure 2.17):

1. Select a normalized temperature (this would be accomplished by an appropriate code which loops over a series of temperature values):

$$\Theta = 0.29029 \text{ (corresponding to } 765.2^{\circ}\text{C}).$$

2. Locate abscissa value ($\frac{x}{2\sqrt{t}}$) corresponding to Θ :

$$\frac{x}{2\sqrt{t}} = 0.012024 \text{ m/h}^{\frac{1}{2}}, \text{ i.e. } \Theta(0.012024) = 0.29029$$

3. Locate corresponding abscissa for the error function ($\frac{x}{2\sqrt{\alpha t}}$):

$$\frac{x}{2\sqrt{\alpha t}} = 0.263218, \text{ i.e. } \text{erf}(0.263218) = 0.29029$$

4. Compute the thermal diffusivity by division of the two abscissa values:

$$\alpha = \left(\frac{0.012024}{0.263218}\right)^2 \text{m}^2/\text{h} = 2.087 \times 10^{-3} \text{m}^2/\text{h} \text{ (or } 5.797 \times 10^{-7} \text{m}^2/\text{s})$$

Note: To be consistent with Schurman's reported data, *hours* were used as the unit for time in figure 2.17 . The results could equally well have been presented with *seconds* as the time unit; however, such a change would have reduced the clarity of

the figure concerned.

The resulting thermal diffusivity (curve II) as compared with the finite element input (curve I) is shown in figure 2.18. Clearly a significant error occurs. Except for a very narrow temperature range, while the body is still at a fairly uniform temperature throughout, all relative errors in the computed diffusivity are well above 10%. The error reaches a maximum of about 75% near 600°C and finishes around 72% at the limit of figure 2.18. Schürman's method overestimates the thermal diffusivity significantly for the bulk of the temperature range. For locations farther away from the interface where temperatures remain fairly low, the thermal diffusivities are somewhat underestimated.

2.3 Accuracy Assessment by the Least Square Method

The method of minimizing the sum of the square of an error is a very basic yet robust approach. It is well established for fitting any kind of data. Its strength lies in its complete independence from the geometry or dimensionality of the problem. It is very general and potentially applicable to any casting situation. The only need is a series of thermocouples for temperature measurements. Given its promise, this method was examined more closely. The examination focused on one dimensional heat flow. Good results were produced in the case of constant thermal properties. Several approaches for the temperature dependent thermal diffusivity case were considered. As will be shown, none were successful.

The basis for this method is similar to all data analysis or curve-fitting: to minimize the square of the error between the computed and the measured results.

For the current application, the error expression appears as follows:

$$\epsilon(\alpha) = \sum_x \sum_t (\hat{T}(x, t) - T(x, t, \alpha))^2 \Delta t \quad (2.12)$$

with:

$\hat{T}(x, t)$ measured temperature at location x at time t
 $T(x, t, \alpha)$ computed temperature with an estimated α

Application of this method would commence by placing a series of thermocouples at known distances from the casting/mold interface to provide the measured temperature field $\hat{T}(x, t)$. The computed temperature field, $T(x, t, \alpha)$, for the same locations and times can be obtained by numerical methods or, in the simplest case, by analytical means if these are available. The computations of $T(x, t, \alpha)$ would be carried out using a series of trial diffusivity values, α . For each location and time step, the error $\epsilon(\alpha)$ can be computed from the summation expressed by equation 2.12. Minimum error values are obtained for the thermal diffusivity which best matches the actual value. Since steps are taken over discrete trial diffusivity values, this method is necessarily limited in accuracy by the size of the steps taken. When only constant thermal properties are involved, the application is simple and should yield good results. The temperature dependent case is much more difficult to evaluate.

2.3.1 Analytical case

In the first instance, this method was tested using conditions for which an analytical solution exists. The one-dimensional semi-infinite heat conduction problem is used. Equation 2.2 will be used to compute a simulated experimental temperature field. Since this is a very simple case with precisely known conditions, the present method should provide good results.

Figure 2.19: Error Curve: ϵ vs. α for analytical case

A semi-infinite solid extending from a plane starting surface at $x=0$ m is considered. Its initial temperature is $T_i=350^\circ\text{C}$. At time $t=0$ sec a surface temperature of $T_o=650^\circ\text{C}$ is imposed and maintained. A constant thermal diffusivity $\alpha=6\times 10^{-6}$ m^2/s is used. Temperatures at nine equally spaced locations from $x=0.005$ m to $x=0.045$ m are monitored. The complete summation over equation 2.12 will yield the single curve shown in figure 2.19. It is clear from this figure that the minimum correctly determines the experimental diffusivity. As expected, the minimum error for this case was zero at the thermal diffusivity of $\alpha=6\times 10^{-6}$ m^2/s .

2.3.2 Temperature dependent thermal property case

It is convenient to describe the temperature dependent diffusivity as a function expanded about some mean temperature, $\bar{T}$, for example:

$$\alpha(T) = \alpha_0 + \alpha_1(T - \bar{T}) + \alpha_2(T - \bar{T})^2 + \dots$$

with:

$\alpha(T)$	the functional representation of the actual thermal diffusivity
$\alpha_0, \alpha_1, \alpha_2$	the required constants
T	temperature

The objective would then be to compute, by means of equation 2.12, each of the constants α_0 , α_1 , α_2 successively. Higher order constants are more difficult to determine accurately. In the present case, the quadratic constant was found to be zero.

To apply this method, a simulated experimental temperature field is first computed with a known temperature dependent thermal diffusivity using FEA. The approximation to α_0 , denoted by α'_0 , can be readily obtained by successively stepping over a series of trial diffusivity values. By comparing the thermal histories for each trial diffusivity with the experimental data using equation 2.12, α'_0 is obtained as the value which produces the smallest error, $\epsilon(\alpha)$. This provides a mean value to the thermal property over the temperature range considered.

The difficulty in determining α'_1 to estimate the linear constant is compounded by the problem of selecting a proper value for $\bar{T}$. Lacking other alternatives, a simple choice would be to select as the mean value, $\bar{T}$, the average of the temperature range involved during the analysis period. Figure 2.20 illustrates the result from one simulated case where the experimental diffusivity varies linearly with temperature. The pouring temperature ranged between $20^\circ C$ and $856^\circ C$; $\bar{T}$ was therefore taken as $438^\circ C$. Shown in the figure are α'_0 and $\alpha'(T)_1$ computed by the least square method as well as the actual $\alpha(T)$ used.

In the case of the quadratic variation with temperature this procedure becomes even more uncertain. Figure 2.21 is the result from one particular case. Shown are the actual diffusivity as well as the constant α'_0 and the linear function $\alpha'(T)_1 = \alpha'_0 + \alpha'_1(T - \bar{T})$ computed by the least square method. The temperature ranged

Figure 2.20: Results for linear variation in actual diffusivity: α'_0 is the least square computed best fit for constant term; $\alpha'(T)_1$ is the least square computed best fit linear equation; $\alpha(T)$ is the actual linear diffusivity

from a minimum 20°C to a maximum 803.6°C ; again the average over this range (412.8°C) was used as $\bar{T}$. Of interest here is that the quadratic term α'_2 could not be found by this method. In fact any deviation from the sloping line $\alpha'(T)_1$ increased the error, $\epsilon(\alpha)$.

A second approach with this method was to consider each nodal location separately. Since nodes further from the casting/mold interface would heat less in the same time frame, any minima computed by equation 2.12 at individual locations would be expected to reflect these different temperature ranges. The thermal diffusivities so computed should then correspond to the various temperature conditions experienced at each individual nodal location. Figure 2.22 shows the thermal diffusivity corresponding to the minimum $\epsilon(\alpha)$ for each of eight nodal locations plotted against the mean and maximum temperatures for each respective location. Also shown is the actual linear thermal diffusivity used to generate the experimental

Figure 2.21: Results for quadratic variation in actual diffusivity: α'_0 is the least square computed best fit for constant term; $\alpha'(T)_1$ is the least square computed best fit linear equation; $\alpha(T)$ is the actual quadratic diffusivity

thermal history. In this case the least square method overestimates the thermal diffusivity.

The last approach taken with this method involved partitioning an experimental thermal history. The partitions were selected in such a manner that the temperature variation during each partition was small enough to consider the thermal property as roughly constant. Application of the least square method over each partition successively would yield a series of diffusivity values (representing mean values over each of the temperature ranges). Since the partitioning was performed on the basis of temperatures, each partition had associated with it a mean temperature. The diffusivities obtained for each partition were then related to this mean temperature. One problem with this method is the large temperature range measured by the thermocouples, even when only sets of three are considered. This undermines the partitioning process which relies on sufficiently small temperature ranges. Three

Figure 2.22: Thermal diffusivity for multi-node approach

cases were examined. Regarding the first as the standard case, each of the latter two were attempts to reduce the temperature difference between the three thermocouples examined. Case 2 achieves this by simply using three thermocouples located closer to the casting/mold interface. Case 3 does the same by using a shell mold with an insulated exterior; the insulation would cause the temperature of the outermost node to rise somewhat and narrow the temperature range among the three nodes. It should be noted that cases 1 and 2 represent the same experimental conditions but with different thermocouple locations, while case 3 represents a different set of experimental conditions. Figure 2.23 compares the resulting curves for these separate cases against the actual thermal diffusivity used in the experiment.

In each case a set of three thermocouples near the casting/mold interface was examined. In the first case three thermocouples at 0.005, 0.010, and 0.015 m from the interface were used. A 0.05 m thick mold with a chilled exterior boundary was modelled in this case. In the second case the three thermocouples were moved closer

Figure 2.23: Thermal diffusivity for history partition approach: case 1 is the standard case with three thermocouples at 0.005 m , 0.010 m and 0.015 m from casting/mold interface with a chill boundary at 0.075 m ; case 2 positions the thermocouples closer to the casting/mold interface at 0.0025 m , 0.00375 m and 0.005 m ; case 3 has thermocouples at 0.005 m , 0.010 m and 0.015 m from casting/mold interface with an insulated boundary at 0.015 m

to the interface at 0.0025, 0.00375, and 0.005 m ; all other conditions remained the same as the first case. Since this resulted in smaller temperature differences among the three thermocouples, an expected improvement is noted. However, such accurate thermocouple placement is impractical and difficult to achieve. In the final case, the thermocouples were again placed at 0.005, 0.010, and 0.015 m from the interface. This time, however, a 0.015 m thick shell mold with a perfectly insulated exterior boundary was examined. This also narrowed the temperature range among the three thermocouples involved. The results again improved, but employed conditions which are not practical in reality. Even with these modifications, the method failed to retrieve the temperature dependent thermal diffusivity correctly. The error was particularly large at higher temperatures. The solidification of castings will be heavily influenced by the high temperature properties of the mold. Thus, failure to accurately determine the high temperature properties is particularly disappointing.

Chapter 3

Solidification Algorithms

Three models were used in the simulations to account for the evolution of latent heat: two latent heat models and the Rappaz model. The first latent heat model is a very simple model and is only briefly described. Of the three models, the second latent heat model is of greatest practical interest and will be discussed in most detail. While it is an equilibrium model which does not deal with microstructural issues, it does produce results which differ little from those of the more complete model of Rappaz. Because of its minimal input requirement, the second latent heat model is easier to apply than the Rappaz model. The Rappaz model provides a more complete description of equiaxed dendritic solidification. It is more complex, however, and potentially difficult to use and expensive to run.

Both latent heat models are equilibrium models. Equilibrium implies a process slow enough that all chemical reactions are completed such that minimum free energy levels are attained. Alternatively, in solidification it would imply that any solute diffusion would have to occur very rapidly. This is rarely achieved and therefore the two latent heat models must be considered approximate. For example, the onset of solidification in real castings usually occurs close to but slightly below the melting point or the equilibrium liquidus temperature. Such undercooling would not be reflected by equilibrium models. Recalescence during solidification which occurs when the latent heat is being evolved more rapidly than it is conducted away is also not captured by equilibrium models.

With regard to the equilibrium models [9], the four possible stages during the

cooling of an alloy are described as follows:

1. Stage I: Pre-solidification

A liquid region, $T \geq T_L$:

$$f_s = 0$$

$$\Delta f_s = 0$$

$$\Delta T = \Delta H / C_p$$

2. Stage II: Primary solidification

A two-phase region consisting either of liquid and primary α or liquid and primary β , $T_L > T > T_S$ (This stage does not exist when $f_s|_{T=T_S} = 0$):

$$0 < f_s < f_s|_{T=T_S}$$

$$\Delta H = C_p \Delta T - L \Delta f_s$$

3. Stage III: Eutectic solidification

A three-phase region consisting of liquid, α and β phases at the eutectic temperature, $T = T_S = T_E$ (This stage does not exist when $f_s|_{T=T_S} = 1$):

$$f_s|_{T=T_S} \leq f_s < 1$$

$$\Delta f_s = -\Delta H / L$$

$$\Delta T = 0$$

4. Stage IV: Post-solidification

The solid region, $T < T_S$:

$$f_s = 1$$

$$\Delta f_s = 0$$

$$\Delta T = \Delta H / C_p$$

with:

T temperature

subscripts L, S respectively: liquidus, solidus

f_s	fraction of solid
H	enthalpy
C_p	specific heat
L	latent heat of fusion
Δi	indicates an increment in i
α, β	indicate the two primary phases of a binary alloy

The first and fourth phases, when the casting is either fully liquid or solid, represent simple heat diffusion problems. These are easy to deal with and are not the focus of the solidification models. The first latent heat model essentially describes stage 3 when eutectic compositions are involved. The second latent heat model describes stages 2 and 3. The Rappaz model simulates solidification occurring during stage 2 as well.

The usual solidification problem is to determine a temperature and fraction of solid (T_2 and f_{s2}) from the temperature and fraction of solid (T_1 , f_{s1} , H_1 , H_2) computed at the previous time step together with the enthalpy values (H_1 , H_2).

3.1 The first latent heat model

This is the simplest of the three models and is appropriate for pure materials and materials of eutectic compositions where solidification occurs at a single temperature. It really is only a special case of the second latent heat model but will be regarded as a separate model for the purpose of this discussion. The latent heat is evolved at a constant temperature as would happen with a pure metal or a eutectic alloy. A smooth solidification front is implied. The casting is considered fully liquid ($f_s=0$) above the melting point (or eutectic temperature for eutectic alloys) and fully solid ($f_s=1$) below it.

At the melting temperature, in the two phase region for a pure material (or the

three phase region at the eutectic temperature for eutectic alloys), the computations follow those described in stage 3 above. With ΔH computed by the FEM thermal analysis and used as input to the model, the fraction of solid can easily be obtained. The temperature during this stage remains constant. When the fraction of solid reaches unity, all latent heat has been evolved and the temperature is allowed to drop once more.

3.2 The second latent heat model [9]

This model relates the fraction of solid and temperature, both functions of enthalpy, by virtue of the equilibrium phase diagram. The enthalpy formation, with notation as before, is expressed as:

$$\Delta H = C_p \Delta T - L \Delta f_s$$

can be rewritten as:

$$\Delta f_s = \frac{\Delta H}{C_p x - L}$$

with: $x = \frac{\Delta T}{\Delta f_s}$

Now, $f_s = f_s(x) = f_{s1} + \Delta f_s = f_{s1} + \frac{\Delta H}{C_p x - L}$

and, $T = T(x) = T_1 + \Delta T = T_1 + \frac{\Delta H x}{C_p x - L}$

The lever rule for the equilibrium phase diagram determines:

$$f_s = F_s(T) = \frac{C_L(T) - C_o}{C_L(T) - C_S(T)}$$

with:

C_o bulk composition of alloy

$C_L(T)$ liquidus concentration at temperature T

$C_s(T)$ solidus concentration at temperature T

The function which relates f_s and T can be stated as:

$$\Psi(x) = f_s(x) - F_s(T(x)) = 0$$

This equation can be solved numerically by such root finding algorithms as the Newton-Raphson method. Given an initial guess for x , $x^{(0)}$, estimates for the roots of $\Psi(x)$ are easily found from:

$$x^{(n+1)} = x^n - \frac{\psi(x^n)}{\psi'(x^n)}$$

where n and $n + 1$ indicate successive iterations. Usually a mean value for x is used as a starting value:

$$x^{(0)} = \frac{T_S - T_1}{f_s|_{T=T_S} - f_{s1}}$$

Only 2-4 iterations are necessary for tolerances of 10^{-6} . The results of this model for an Al-7wt%Si casting compare very well with those obtained by the Rappaz model and require roughly 90% less CPU time for the solidification code alone. When coupled with FEM thermal analysis, this solidification model consumes a nearly negligible fraction of the total CPU time.

3.3 The Rappaz Model [10,11,12]

Since it is not within the scope of this thesis to fully describe this model, only a brief qualitative description will be provided here. More detail can be found in [10, 11, 12] and Appendix A.

Rappaz models the microstructural evolution during equiaxed solidification to obtain more realistic results for non-eutectic alloys. For these materials microsegregation results in a mushy zone within which the solid/liquid interface has a very

complex shape. Latent heat release in this case is directly related to the evolution of the fraction of solid, $f_s(t)$. Macroscopic solidification models which compute temperature fields during solidification usually assume that the evolution of latent heat depends only on the temperature. Rappaz, in his model, provides a more thorough treatment of the microstructure by including nucleation and growth kinetics while maintaining thermal and solute balances.

Four phases, described in [10], are involved in this model: (1) nucleation, (2) spherical growth, (3) dendritic growth, and (4) impingement. The fourth phase developed by [17] actually corresponds to stage III of solidification described earlier. It is assumed that upon nucleation the equiaxed grain is spherical and maintains this geometry through the second phase. Both the nucleation and spherical growth phases involve the growth of a completely solid sphere. The latter two phases retain this simple geometry by assuming grain growth within a spherical volume occupied by liquid and solid of various fractions depending on the maturity of the grain. Figure 3.1 describes the terminology for the developing grain. Each phase essentially tracks the fraction of solid formed and together with the energy equation computes the resulting temperature change. While this computation is straightforward for the first and fourth phase; it is more complicated for the middle two phases. The FEM heat equation:

$$C(\frac{T_3 - T_1}{\Delta t}) - L(\frac{f_{s3} - f_{s1}}{\Delta t}) + K[\theta T_3 + (1 - \theta)T_i] + Q = 0$$

with:

$C, K, \text{ and } L$	capacitance, stiffness and conductivity matrices
T_1, T_3	temperature at start and end of time step
f_{s1}, f_{s3}	fraction of solid at start and end of time step
θ	integration scheme parameter ($0 \leq \theta \leq 1$)

Figure 3.1: 1. R_t - Radius of total grain; 2. R_g - Radius of grain envelope; 3. Liquid inside grain envelope; 4. Solid inside grain envelope ; 5. Liquid outside of grain envelope. The internal fraction of solid is defined as $f_i = \text{volume}_4 / \text{volume}_2$. The fraction of grain is defined as $f_g = \text{volume}_2 / \text{volume}_1$. The fraction of solid is then $f_s = f_i * f_g$. Source: [10].

is a non-linear equation such that a residual method has to be employed to solve for the unknown temperature T_3 . With the fraction of solid computed as indicated by each phase, this equation can be solved iteratively until the residual in the computed temperature becomes sufficiently small.

A large number of parameters are required for this model. The most difficult values to obtain are those needed for a complete description of the microstructure in the Rappaz model. These must be obtained experimentally and are generally not well known for most casting alloys. Four parameters are needed to describe nucleation conditions. These indicate: (1) The maximum undercooling to activate all nuclei, (2) The undercooling for peak nucleation rate, (3) The maximum density of nuclei, and (4) The standard deviation for the continuous distribution describing the nucleation sites. Five parameters are needed to describe the critical grain radius necessary for stable growth. This is determined from a balance between the volume and surface free energy of the growing grain at various temperatures. The first of these five indicates a reference temperature; the remaining four are constants for

a cubic polynomial relating the critical radius to temperature. Two more parameters are needed to describe the velocity of the dendrite tip advance as a function of undercooling. In addition, eight parameters are required to describe the alloy used. These are easily obtained and are as follows: (1) The bulk composition of the alloy, (2) The eutectic composition of the alloy, (3) The latent heat, (4) The solute diffusivity, (5) The eutectic temperature, (6) The melting point of the pure metal, (7) The slope of the liquidus line, and (8) The equilibrium partition/distribution coefficient (or slope of the solidus line).

Further detail on the four phases of the Rappaz model is included in Appendix A.

Chapter 4

Software Validation

This chapter deals with the validation tests conducted on an FEM-based casting software developed at Carleton. The development of any simulation software has as its ultimate goal the accurate prediction of the physical event being modelled. Prior to extended use, the software must first pass through the critical process of validation. This is a time consuming task as it involves many tests on very simple problems, initially, followed by many more tests on more complicated problems toward the end. Software validation involves two main stages. In the first, one must ensure that the software correctly models the underlying physics for its intended class of problems. In the second, and often more difficult stage, one must determine how well the software simulates real physical events.

The primary stage is the more fundamental of the two. It validates the software for its intended class of problems. Basically this stage verifies that all governing differential equations are correctly solved. This is accomplished by testing the software on problems for which analytical solutions exist. Analytical solutions are usually idealized cases of more complex physical problems to which simplifying assumptions have been applied. This, along with the precise definition of the analytical problem leads one to expect very accurate results. Geometry, initial conditions, boundary conditions, material properties are known exactly. Any discrepancies between the predicted and analytical results would be due to errors inherent in any numerical computation. In FEM, among others, the choice of mesh, time step, type of element, and time integration scheme contribute in varying degrees to any numerical error.

Comparison with analytical results answers fundamental questions about the software's ability to solve problems governed by specific differential equations. The conditions imposed in analytical solutions are usually highly simplified and may not accurately portray realistic conditions.

The more important step in software validation is to compare the numerical predictions with physical measurements from real experiments. These experimental cases may be taken from published literature. In the present application, thermal histories, temperature distributions, or solidification patterns measured experimentally form the basis for comparison. Comparisons made with experimental results are more difficult to interpret than those made for analytical cases. Agreement is usually poorer due to the inaccuracies inherent in any experimental procedure. Even when measurements are made with extreme care, variations in the material properties will affect experimental measurements. In addition, the experimental conditions may not have been well defined; boundary or initial conditions may not be specified clearly or may be too complex to simulate exactly. As well, assumptions made in the numerical simulation may affect the predictions; for example, heat flow may have to be reduced by one or more dimensions in the numerical analysis. Then, of course, errors are introduced in the numerically discrete description of the real object represented by the finite element mesh. Mesh selection and element type are further factors of concern. There may also be aspects of the physics which the software may not be designed to capture. In the present version of the software, for example, fluid flow is not considered. The current software also simulates pouring conditions by prescribing a constant initial temperature throughout the casting at the starting time, $t=0$ seconds. This, of course, is not entirely realistic since temperature variations are formed throughout the casting prior to complete filling and also because the mold will have heated during the filling period.

A further limitation in the software is the way in which the gap formation at the casting/mold interface is treated. Upon pouring good contact between the fluid

metal and the mold wall is established to produce a high contact conductance. However, upon solidification, shortly after the first solid skin develops at this interface, the casting contracts to create a gap. In addition, the mold may also expand away from or toward the casting, further altering the contact conductance. This matter is complicated further by gap size variations due to geometry. The heat transfer at the interface is further influenced by the surface preparation of the mold wall and the dissolved gas content of the casting. Proper treatment of this issue must include the stress and deformation of the casting and mold as well as the usual thermal analysis. In the present study a very simplified approach has been taken. The contact conductance at the casting/mold interface is assumed to vary linearly from a high value at some upper temperature threshold to a low value at a lower temperature. The temperature on the casting side of the interface is used to determine these values. This implies that the gap size is governed purely by temperature. This of course is not an accurate representation of the physical situation.

Selection of experimental cases at this stage also poses some difficulty. Reported data is often incomplete; in other cases, while completely documented, the problem may simply be too complex for simulation. In some cases critical material properties may simply not be known. Four cases are examined; the first is an analytical case while the remaining three come from experiments recorded in published literature.

4.1 Analytical case

The analytical case taken from [18] assumes that heat flow is one dimensional, mold metal interface resistance is negligible, and the mold is very thick. The problem is further simplified by assuming zero superheat and constant thermal properties. The mold extends from $x=0$ to $x=-\infty$ and the casting extends from $x=0$ to $x=\infty$. Figure 4.1 shows the problem examined.

The governing differential equation is the one-dimensional heat equation de-

Figure 4.1: Schematic of the analytical solidification problem

scribed earlier. The boundary conditions are: at $x = -\infty$, $T = T_i$ and at $x = \infty$, $T = T_M$. The initial conditions are $T = T_i$ at $x < 0$ and $T = T_M$ at $x > 0$. The initial temperature of the mold is T_i . T_M is the initial temperature of the casting set at the melting temperature. At the liquid/solid interface the Stefan condition governs the release of latent heat:

$$k \left(\frac{\partial T}{\partial x} \right)_{x=S} = L \rho_s \frac{\partial S}{\partial t} \quad (4.1)$$

with:

S	thickness of solidified casting - m
L	latent heat of fusion - J/kg
ρ_s	density of the solidified casting - kg/m^3
k	thermal conductivity - $W/(m \cdot C)$
t	time - sec
x	location from casting / mold interface - m

The solution to equation 4.1 is given by:

$$S = 2\gamma \sqrt{\alpha_s t}$$

where α_s is the thermal diffusivity of the solid. The parameter γ can be determined

Figure 4.2: Analytical solidification case: FEM mesh

from:

$$\gamma \exp(\gamma^2) \left(\sqrt{\frac{k_s \rho_s c_s}{k_m \rho_m c_m}} + \operatorname{erf}(\gamma) \right) - \frac{c_s}{L \sqrt{\pi}} (T_M - T_i) = 0$$

where the subscripts m and s indicate the mold and solid respectively. The interface temperature is determined from:

$$T_{int} = T_i + \frac{T_M - T_o}{1 + \frac{k_{mold}}{k_s} \sqrt{\frac{\alpha_{mold}}{\alpha_s}}}$$

Finally, the temperature distribution in the mold is solved as:

$$T(x, t) = T_{int} + (T_M - T_i) (\operatorname{erf} \gamma)^{-1} \operatorname{erf} \frac{x}{2\sqrt{\alpha t}} \quad \text{in the casting } (x > 0), \text{ and}$$

$$T(x, t) = T_{int} + (T_{int} - T_i) \operatorname{erf} \frac{x}{2\sqrt{\alpha t}} \quad \text{in the mold } (x < 0).$$

Figure 4.2 shows the mesh used in the numerical analysis with the casting and mold as indicated. The mesh was insulated on all external boundaries. The casting is 0.0889 m thick and the mold is 0.6111 m thick resulting in a total 0.7 m long mesh. The problem is one dimensional with thermal gradients existing only along the longitudinal axis. The analytical solution is valid for the case of an infinitely thick casting and mold. This condition is satisfied so long as the thermal disturbance has not yet propagated to either the extreme end of the casting or mold. The casting was given an initial temperature of 660°C and the mold was initialized at 350°C. Material properties were chosen to simulate an aluminum casting in a

Figure 4.3: Analytical solidification case: Temperature distribution at 100 seconds

cast iron mold. Constant material properties were used for the casting and mold. The thermal conductivity and volumetric specific heat of the casting were taken as $81.98 \text{ W/(m } ^\circ\text{C)}$ and $2.99 \times 10^6 \text{ J/(m}^3 \text{ } ^\circ\text{C)}$ respectively; for the mold, values of $30.51 \text{ W/(m } ^\circ\text{C)}$ and $4.56 \times 10^6 \text{ J/(m}^3 \text{ } ^\circ\text{C)}$ were used. Since the analytical case has a negligible interface resistance, a contact conductance of $1 \times 10^6 \text{ W/(m}^2 \text{ } ^\circ\text{C)}$ was used.

Figures 4.3 and 4.4 compare the computed and analytical temperature distributions at two different times. The extent of the mold temperature profile is only indicated up to 0.2 m for clarity; the actual mold used is much thicker. Figure 4.3 shows the temperature profile at 100 seconds after pouring. The casting has partly solidified as indicated by the increased gradient below the 660°C pouring temperature. At a later stage (1100 sec) in figure 4.4 the casting has almost completely solidified. Beyond this point, of course, the temperature will drop at the extreme end of the casting and the analytical solution will no longer be valid.

The agreement between the results is very accurate. The numerical computation correctly predicts the constant interface temperature during solidification. The

Figure 4.4: Analytical solidification case: Temperature distribution at 1100 seconds

predicted time for complete solidification at 1138.9 seconds also compares very well with the analytical time of 1130.2 seconds. The largest discrepancy between the analytical and numerical solutions occurs at the interface where an infinitely large contact conductance is assumed; a larger contact conductance may improve the results. Some discrepancy from mesh discretization and time integration is to be expected with any numerical solution.

4.2 Al-7Si Casting

Lee *et al* [13] investigated the combined influence of feeder size and casting length on the feeding behaviour of Al-7Si-0.3Mg alloy. A series of casting experiments were performed in which riser size and casting length were varied. One of these experiments for which results were well documented was selected for the present validation test. The casting and rigging are shown in the FEM mesh in figure 4.5. This case had a riser height of 0.012 m with a 0.08 m diameter. The casting itself

Figure 4.5: Al-7Si casting: FEM mesh

is a flat rectangular plate measuring 0.14 *m* wide, 0.02 *m* high, and 0.25 *m* long. Six thermocouples were introduced into the riser center and mold cavity, at equal intervals along the longitudinal axis of the casting, at mid-height. Thermal histories for these thermocouples as well as solidification times along the longitudinal axis of the casting were reported.

The mesh used for the FEM simulation (figure 4.5) contains some 5080 elements. The figure shows that the mesh is rather coarse in the region of the plate where the thermocouples are located. The plate is only four elements thick. Initially the simulation was performed with a constant heat transfer coefficient representing the combined effect of the mold and surroundings. The same case was also run with a full mold attached; 23690 elements were needed in this latter case. This increased the execution time nearly six times from roughly six hours to about thirty-six hours. Results from both cases are described.

The Rappaz model was used for this investigation because the solidification mode of this alloy corresponds to that modelled by Rappaz. Except for a narrow region at the mold wall, aluminum alloys cast into sand molds undergo primarily equiaxed dendritic solidification. This is especially true when the alloy has a long freezing range and when little superheat is involved. Although the actual pouring temper-

Bulk alloy composition	7.0 wt% Si
Eutectic concentration	12.6 wt% Si
Latent heat of fusion	$9.5 \times 10^8 \text{ J/m}^3$
Solute diffusivity	$3.0 \times 10^{-9} \text{ m}^2/\text{s}$
Eutectic temperature	566.0°C
Melting point of pure metal (aluminum)	660.0°C
Partition coefficient	0.117
Quadratic coefficient for dendrite velocity	2.904×10^{-6}
Cubic coefficient for dendrite velocity	1.488×10^{-6}
Reference temperature for critical grain radius	660.0°C
Constants for critical radius polynomial	0.0
Max undercooling to activate all nuclei	12.0°C
Undercooling for peak nucleation rate	6.0°C
Maximum density of nuclei	$1.0 \times 10^9 \text{ m}^{-3}$
Standard Deviation of nucleation distribution	2.0°C

Table 4.1: Solidification parameters for Al-7Si casting

ature was 700°C , most of the superheat was dissipated before reaching the casting plate. As noted from the thermal histories, the peak temperatures in the casting varied from about 615°C to 605°C . This alloy was particularly suited for the Rappaz model since most of the input parameters for this model had been made available by Rappaz [12]. The data used is shown in table 4.1.

4.2.1 Casting without mold

Just after pouring the temperature gradients in the mold are very large but decrease rapidly as the casting cools and the mold heats up. Heat flux from the casting to the mold decreases from large initial values in a logarithmic fashion. To correctly capture

Figure 4.6: Al-7Si casting without mold: Thermal history at 0.025 *m* from free end

this behaviour, a time varying equivalent heat transfer coefficient should have been used. Since this option was not available it was necessary to use a constant value. A heat transfer coefficient of 50 $W/(m^2 C)$ was used for the present test.

Figures 4.6, 4.7, and 4.8 compare the predicted and experimental histories for three thermocouples at 0.025, 0.125, and 0.225 *m* from the casting free end. Figure 4.9 shows the predicted and experimental solidification times for the casting. Good agreement has been obtained.

The differences between the predicted and measured results could come from several factors. Most notable for this case is, of course, the constant heat transfer coefficient used to model the mold. Being too low for early times and too high for later times results in underestimated heat flow at the beginning and overestimation towards the end. This should cause some delay in cooling at earlier times and excessive cooling rates at later times. The thermal histories reflect this. This explains the delay in the solidification end times toward the free end of the casting, the first portion to solidify. A second reason for the discrepancy is the fact that

Figure 4.7: Al-7Si casting without mold: Thermal history at 0.125 *m* from free end

Figure 4.8: Al-7Si casting without mold: Thermal history at 0.225 *m* from free end

Figure 4.9: Al-7Si casting without mold: Solidification start and end times

fluid flow upon filling and during solidification was neglected. The former results in some cooling of the melt as it fills the mold cavity. In fact peak temperatures of the experimental thermal histories indicate a decrease toward the casting free end; this varies roughly from 615°C to 605°C . The uniform pouring temperature of 620°C for the numerical computation would certainly delay the solidification times for the portion of the casting to solidify first. This is consistent with figure 4.9. The predicted early solidification end times near the riser can also be explained by the fact that fluid flow during solidification was neglected. Shrinkage occurring in the first portions of the casting solidify will draw hot liquid metal into the plate from the riser. This causes a delay in the solidification of the casting in this region.

4.2.2 Casting with mold

In the second examination a full mold was attached to the FEM mesh shown previously in figure 4.5. 23690 elements were used this time and the execution time

Figure 4.10: Al-7Si casting with mold: Solidification start and end times, case 1

increased roughly six fold. Thermal properties for a silica sand were used. The contact conductance at the casting/mold interface was set to vary linearly from 100 to $1000 \text{ W}/(\text{m}^2 \text{ } ^\circ\text{C})$ between a low and high threshold of 500°C to 550°C . Two test cases were considered. In the first test case a pouring temperature of 620°C was used to be in rough agreement with the peak temperatures reported in the casting. In the second test case the actual pouring temperature of 700°C was used.

Comparison of solidification times for the first test case are shown in figure 4.10. The figure shows that both the predicted starting and ending times occur too early. The simulation was run with a uniform 620°C pouring temperature throughout the melt at time $t=0 \text{ sec}$. The mold had an initial value of 20°C . These conditions were chosen to approximate the peak temperatures encountered in the experimental casting (615°C to 605°C). The 5 degree additional superheat resulted from an extrapolation of the reported thermal histories in the casting to the pouring time, $t=0 \text{ sec}$. The initial condition used for the mold was chosen to conform with the reported initial temperature of the mold at ambient temperature. Using an artificially low

Figure 4.11: Al-7Si casting with mold: Thermal history at 0.025 *m*, case 2

contact conductance does improve the agreement with experiment.

The results indicated that heat was being extracted from the casting too rapidly. This could be caused by inaccurate thermal properties or contact conductance values; comparison with other sources indicated that neither of these was the case here. The more likely cause was the initial temperature. The choice of initial temperature for the casting and mold was in fact at odds with the experimental condition. The experimental melt was poured at $700 \pm 5^\circ\text{C}$. This additional superheat, while dispersed quickly, serves to preheat the mold during solidification. In fact, solidification no longer proceeds into an initially cold mold. This, of course, significantly decreases the thermal gradients at the casting/mold interface, hence retarding the heat extraction. Indeed it is very bad practice to use an initial temperature below the pouring temperature since this energy must be included in the analysis.

To test this hypothesis a second case was analyzed with a 700°C initial temperature in the melt; all other conditions were retained from the first case. Figures 4.11, 4.12 and 4.13 compare the predicted and experimental thermal histories at 0.025.

Figure 4.12: Al-7Si casting with mold: Thermal history at 0.125 *m*, case 2

Figure 4.13: Al-7Si casting with mold: Thermal history at 0.225 *m*, case 2

Figure 4.14: Al-7Si casting with mold: Solidification start and end times, case 2

Figure 4.15: Al-7Si casting with mold: Solidification contours, case 2

0.125, and 0.225 *m* from the casting free end. It can be seen how rapidly the superheat is lost. Figure 4.14 compares the predicted and experimental solidification times. Very good agreement is observed in the solidification times. The agreement is very good considering the scatter in reported thermal properties and the crudeness of the contact conductance model used in the FEM computations. One must also consider the difference in the definition of complete solidification. Lee *et al* in their paper defined a solidus temperature of approximately 556°C to signify the end of solidification. In the present models the completion of solidification is determined by the solidus temperature, 566°C in this case. This difference causes the numerical solidification to occur somewhat earlier than expected. Figure 4.15 shows the solidification contours across the casting and riser. They indicate that the casting cools from its outer edges inward; the riser center, correctly, is the last to solidify. This correct prediction of the solidification progression is in itself an important casting design tool.

4.3 Ductile Iron Casting

The second experiment examined here was taken from Bradley and Fung [14]. Their study was aimed at shrinkage prediction in ductile iron castings. Results from their numerical models were also documented.

The geometry and boundary conditions for this case are very simple. The casting, a cylinder 0.04 *m* in diameter and 0.048 *m* high, was held in an open top thermal analysis cup. A single thermocouple was placed at the geometric center of the casting to obtain the thermal history. A commercial, near eutectic ductile cast iron (CE=1.56 based on $CE = \%C + \frac{1}{3}\%Si$) was used. The casting had a uniform initial temperature of 1220°C. Constant thermal properties were also provided; the thermal conductivity and volumetric specific heat of the casting were 29.3 W/(*m* °C) and 4.91×10^6 J/(*m*³ °C) respectively. A latent heat of 1.44×10^9 J/(*m*³) was indi-

Figure 4.16: Axisymmetric FEM mesh for ductile iron casting. (Cross-hatch indicates insulated boundary condition.)

cated. Convective boundary conditions were assumed for the top and sides of the casting. A heat transfer coefficient of $125.5 \text{ W/(m}^2 \text{ C)}$ was used for the open surface at the top and $71.2 \text{ W/(m}^2 \text{ C)}$ for the sides. The base of the casting was considered insulated. An ambient temperature of 20°C was assumed.

Figure 4.16 shows the FEM mesh used for the numerical simulation. Since this was an axisymmetric case, only half the geometry needed to be modelled; the left edge representing the axis of the cylinder, was insulated. The base of the mesh was also insulated. Point A on the left edge of the mesh marks the placement of the thermocouple; the predicted and measured thermal histories for this location were compared in figure 4.17.

The delay in cooling at earlier times and the accelerated cooling rate predicted towards the end may in part be an effect of the constant heat transfer coefficient used to model the thermal analysis cup. In any case, the comparison is quite good.

The numerical analysis used the simple latent heat model. This model simply

Figure 4.17: Thermal history at location 'A' for ductile iron casting

represents the liquid/solid interface with a plane front, which is the case for pure metals, or for alloys under directional solidification and low growth rate or high temperature gradients. Upon reaching the eutectic temperature in the simple latent heat model, the temperature is maintained constant until all the latent heat has been exhausted; at this point the solidification is complete and the cooling curve experiences a sudden sharp drop. This differs from the real casting, especially towards the center of the casting as is the case here, where some undercooling is usually experienced. The real cooling curve describes a balance between the evolution of heat in a sample and the heat transport away from it. As a result the flat plateau at the eutectic indicated by the simple latent heat model does not really occur. Nonetheless, even with this simple model, the agreement is very good.

4.4 Induction Furnace Steel Casting

The final validation test models one of a series of experiments conducted by Bishop *et al* [15]. Their study examined the effect of mold walls of different material properties, mold thickness, moisture content, as well as superheat on the solidification of induction furnace steel.

The bottom gated steel casting had a composition of 0.6% C, 0.5% Mn, 0.3% Si, 0.1% Al. The casting was a simple rectangular prism 0.508 *m* (20 *in.*) high with a square cross section: 0.171 *m* $\times$ 0.171 *m* (6.75 *in.* $\times$ 6.75 *in.*) at the bottom varying to 0.184 *m* $\times$ 0.184 *m* (7.25 *in.* $\times$ 7.25 *in.*) at the top. A series of thermocouples were positioned at mid-height of the casting. Three different mold materials of varying thicknesses were used in the experiment by Bishop *et al*: a gray iron chill, a dry sand, and a green sand.

For the present simulation, results from a dry sand mold test were used for the validation. The sand was an AFS No.80 silica sand (3% water, 3% bentonite, 0.5% cereal, 1.5% dextrine). It was baked at 232°C (450°F) for 16 hours to remove the water content. The results from this test were selected because gap formation and contact resistance have a smaller effect on the thermal history in sand molds than in cast iron molds. Contact conductance values across the gap are not usually well known since they vary with time, position, contact pressure and mold geometry.

The mesh used is shown in figure 4.18. Bishop contends, that the bottom and riser gradients are essentially eliminated at the casting mid-height. Thus only two-dimensional heat flow was considered. The required mesh could further be reduced to the wedge shape shown in figure 4.18 due to existing symmetry. The present results are not as good as those for the previous tests. Solidification starts too early and ends too late. This difference is magnified towards the center of the casting, deviating from the experimental values by about 40% at this location.

While differences between the simulation and experiment are to be expected, the

Figure 4.18: Steel casting: FEM mesh. (Cross-hatch indicates insulated boundary condition.)

magnitude of the present discrepancy cannot be readily explained. Undoubtedly the limitations of the latent heat model contribute to this error. Most notable is the fact that the latent heat model is an equilibrium model which assumes that all alloying elements exist as a stable solution in the parent metal. This is not true and may be of even more practical significance with columnar dendrites. With long columnar dendrites growing inward from the mold wall, significant redistribution of solute will occur during solidification. There will not only be microsegregation laterally but also macrosegregation along the length of the dendrites. Such effects would be emphasized by the long solidification range (roughly 70°C) in the present case. This in turn may contribute to the inaccurate computation of the solid fraction developed at any given time.

The issue of convection or fluid motion during solidification is also not treated in the latent heat model. Convection currents are set up when the hot metal is poured against the much cooler mold wall. The resulting density differences create downward flowing currents near the mold wall and rising currents toward the center of the casting where the metal is hottest. Fluid flow is also induced as the interdendritic liquid begins to solidify and shrink; this should cause increased flow of hot metal from the casting center. These effects are expected to retard solidification. The delayed solidification ending times predicted by the software are therefore not explained by the omission of the fluid flow.

The experimental casting was poured at 1537.8°C (2800°F) with a reported liquidus of 1482.2°C (2700°F); the solidus was approximately 1410°C . Figure 4.19 compares the predicted solidification times of two separate tests against the experimental times. In both cases the initial temperature of the mold was taken as 65°C . The contact conductance in both cases was varied between $300\text{ W}/(\text{m}^2\text{ K})$ and $2000\text{ W}/(\text{m}^2\text{ K})$ for lower and upper thresholds of 1000°C and 1200°C . The first curve labelled as case 1 reports the result for the temperature conditions discussed above ($T_{\text{pour}} = 1537.8^{\circ}\text{C}$, $T_{\text{liquidus}} = 1482.2^{\circ}\text{C}$, $T_{\text{solidus}} = 1410^{\circ}\text{C}$). While these correspond

Figure 4.19: Steel casting: Comparison of solidification times for two different tests against experimental data: case 1 with $T_{pour} = 1537^{\circ}C$, $T_{liquidus} = 1482.2^{\circ}C$, $T_{solidus} = 1410^{\circ}C$; case 2 with $T_{pour} = 1500^{\circ}C$, $T_{liquidus} = 1465^{\circ}C$, $T_{solidus} = 1435^{\circ}C$

to the data reported by Bishop *et al*, marginal improvement was obtained by altering the conditions as follows: $T_{pour} = 1500^{\circ}C$, $T_{liquidus} = 1465^{\circ}C$, $T_{solidus} = 1435^{\circ}C$. The lower pouring temperature resulted in better agreement with the experimental thermal profiles in the casting. The result of this second test is labelled as case 2 in figure 4.19.

Consequent to this, the influence of several parameters on the predicted solidification times was examined. While they do improve the results somewhat, the necessary changes are for the most part unrealistically large and do not sufficiently explain the difference between the predicted and experimental result. The parameters examined will be discussed in relation to case 2 as the standard test; the effects on case 1 should be similar. The parameters examined are as follows: 1) the latent heat, 2) the contact conductance, 3) the thermal conductivity of the liquid and solid

Figure 4.20: Steel casting: Thermal profiles at 1 min. and 50 min.

casting, and 4) the amount of superheat. In all cases reasonably good agreement is obtained for the thermal profiles in the mold. The thermal behaviour in the mold appears to be insensitive to the variables examined. Figure 4.20 compares the predicted thermal profiles for case 2 with the experimental profiles. The earliest and latest reported times (1 min. and 50 min.) are shown in this figure. The mold in this case extends from 0.0889 m (3.5 in.) to 0.1937 m (7.625 in.). The delay in the predicted cooling of the casting is also apparent here; the center of the casting at 0 m has already cooled to 1405°C at $t = 50$ min. while the predicted temperature is still about 1460°C .

Figure 4.21 shows the effect of the latent heat of fusion. The typical value quoted in the literature for cast steel is in the neighborhood of $2 \times 10^9 \text{ J}/(\text{m}^3)$. A reduction to $1.3 \times 10^9 \text{ J}/(\text{m}^3)$ has a large accelerating effect on the solidification ending time and only slightly delays the starting time. The overall delay of the solidification period with increasing latent heat of fusion is correctly reflected by these results.

Figure 4.21: Steel casting: Effect of latent heat of fusion on solidification times

Figure 4.22: Steel casting: Effect of contact conductance on solidification times

Figure 4.23: Steel casting: Effect of casting thermal conductivity on solidification times

Figure 4.24: Steel casting: Effect of superheat on solidification times

Figure 4.22 shows the effect of increasing the contact conductance. Case 1 on this figure was obtained by using the contact condition discussed previously ($300 \text{ W/(m}^2 \cdot \text{K)}$ and $2000 \text{ W/(m}^2 \cdot \text{K)}$ for lower and upper thresholds of 1000°C and 1200°C). Case 2 on the same figure was run with the assumption of negligible interface resistance; a constant value of $50000 \text{ W/(m}^2 \cdot \text{K)}$ was inserted. As can be seen this had only a small effect in accelerating both the solidification starting and ending times. The direction of the change is as expected. The small size of this change confirms the assumption that thermal histories of casting in sand molds are relatively unaffected by interfacial gaps.

Figure 4.23 shows the effect of reducing the thermal conductivity of the liquid metal by 50% while also increasing the thermal conductivity of the solidified metal by 50%. This had a great effect in delaying the solidification starting times. A slight reduction in the solidification ending times was also noted. The reduction in the liquid thermal conductivity had a great effect in delaying the solidification start times; it only slightly delayed the ending time towards the center of the casting. The increase in the thermal conductivity of the solid metal caused minimal delay in the solidification start times while effecting an acceleration of ending times toward the center of the casting.

Figure 4.24 illustrates the effect of varying the pouring temperature. As expected, the additional superheat causes a general delay in the solidification times. Case 1 is the standard test case using a pouring temperature of 1500°C , while case 2 is poured at 1537.8°C with all other conditions remaining the same. This effect agrees well with those observed by Bishop *et al* in their experiments. The two solidification start curves reflect the delay caused by the higher pouring temperature. After an initial short period during which the superheat is released, the rates of the solidification curves become the same. As well, the larger displacement of the ending curves caused by the increased superheat is correctly reflected by these results.

Judging from the previous results, the latent heat value and the thermal conductivity of the casting are the variables with the most significant influence. The contact conductance expectedly has little effect on the course of solidification of the sand casting. Although the lower pouring temperature and altered liquidus and solidus (as shown by case 2 in figure 4.19) resulted in much better agreement between the experimental and predicted results, the resulting modified case no longer reflects the actual casting conditions. As was shown earlier with the Al-7Si casting in section 4.2 one must include the correct superheat to capture the preheating of the mold which occurs in the short time after pouring during which the superheat is dissipated. A final case was considered using the experimentally reported conditions of: $T_{pour} = 1537.8^{\circ}\text{C}$, $T_{liquidus} = 1482.2^{\circ}\text{C}$, $T_{solidus} = 1410^{\circ}\text{C}$. However, in this case the latent heat was reduced to $1.3 \times 10^9 \text{ J}/(\text{m}^3)$ and the thermal conductivity of the liquid was reduced by 50%. The resulting solidification time together with the experimental data are shown in figure 4.25. While the reductions in the latent heat and thermal conductivity of the liquid metal are unrealistic, these changes do demonstrate the sensitivity of the predictions to material properties.

Of the four validation tests reported here, all but this final test agreed well with their experimental counterpart. Part of the difficulty with this last test case is the mode of solidification. This experiment involved columnar solidification over most, if not all, of the seven inch ingot cross section. This mode of solidification with long columnar dendrites and regions of interdendritic liquid extending inward from the mold wall presents particular modelling difficulties. A major problem is due to the equilibrium model used in the simulation. This immediately places uncertainty on the fraction of solid evolved. The difference between the equilibrium and experimental fraction of solid at any time can be quite large. These effects, which are not captured in an equilibrium model, are the result of the micro- and macrosegregation occurring along the dendritic columns and are further complicated by the ensuing local undercooling at the dendrite tips. Figure 4.26, reproduced

Figure 4.25: Steel casting: Effect of decreased latent heat and liquid thermal conductivity on casting poured at $T_{pour} = 1537.8^{\circ}C$ with $T_{liquidus} = 1482.2^{\circ}C$, $T_{solidus} = 1410^{\circ}C$; $L = 1.3 \times 10^9 J/(m^3)$, $k_{liquid} = 0.5 \times \text{reported value}$

Figure 4.26: Comparison of fraction of solid vs. temperature for three models: (1) a linear model (short dashed line), (2) a Scheil model (long dashed line) and (3) the experimentally measured data (solid line). Source: [19]

from [19], illustrates this point for an aluminum based alloy. This figure shows the fraction of liquid against temperature on three different curves: (1) a linear model, (2) a Scheil model, and (3) the experimental measurement. It is expected that the availability of experimental data such as shown by curve 3 in figure 4.26 would improve results.

Given the degree of segregation occurring it is also possible that the latent heat of fusion is not constant, but instead depends on the composition of the solid being formed. Macrosegregation results in different chemical composition at the center than at the surface of the solidified ingot. Thus the total latent heat evolved may be different for volumes at the surface or center. Microsegregation results in local composition differences. Thus the latent heat evolved by a local increment in the solid fraction, Δf_s , may be dependent on the current liquid composition and thus on the fraction already solidified, f_s .

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Chapter 5

Conclusion and Future Work

This chapter discusses the conclusions drawn from the examinations conducted in this thesis as well as the possibilities for future work in this area.

Conclusions:

1. The foremost conclusion to be drawn from the thermal property examination is that a viable in-situ method for the determination of temperature dependent thermal properties does not exist. A review of current literature on the subject revealed that while several methods have been proposed, they fail to be sufficiently accurate or do not work altogether.
2. The finite difference approach can be easily overwhelmed by errors, both due to measurement and due to the finite difference discretization. Generally such an approach will require unusually thick molds or excessive experimentation times to yield results with acceptable accuracy.
3. The least-square minimization method while having the potential to be the most generally applicable method is not successful in the measurement of temperature dependent thermal properties.
4. A variety of in-situ methods can accurately measure temperature independent (constant) thermal property values. These are, however, of little practical value in casting simulation where thermal properties can vary considerably

with temperature. With the wide variety of existing molding sands and the importance of accurate thermal properties required for the simulation and design of castings, this work is far from complete.

5. The second half of this thesis concerned the validation of the solidification code. Results from the various tests indicate that good agreement is generally achieved. It must be remembered that it will be unlikely, except in the simplest of situations, to obtain exact agreement between an experiment and a numerical model.
 - (a) Software predictions for the analytical solidification problem (section 4.1) were very accurate.
 - (b) FEM computed thermal histories and solidification times for the Al-7%Si casting using the Rappaz model were in good agreement with the experimental results. Any differences were explained (section 4.2).
 - (c) The prediction of the thermal history using the simple latent heat model for the ductile iron casting (section 4.3) was good.
 - (d) While the the second latent heat model did not accurately compute the solidification times for the steel ingot (section 4.4), general solidification behaviour was properly predicted. Underlying difficulties with this particular case were discussed. Future work on the fluid flow and contact conductance are anticipated to improve results for such cases.
6. As expected, an increase in the latent heat of fusion prolongs the overall solidification period. This happens as a result of slight delays in the solidification start times and longer delays in the solidification ending times.
7. While increased contact conductance is expected to slightly accelerate both the solidification start and end times, it has been confirmed that this effect

is minimal when sand castings are involved. This is due to the fact that the thermal resistance of molding sands is already very large.

8. Additional superheat delays both the solidification starting and ending times; the delay on the ending times is larger. Essentially the higher pouring temperature results in a shift of the solidification start and end curves to later times. This is in agreement with experimental observation.
9. A reduction in the thermal conductivity of the liquid causes a greater delay in the solidification start time than the end time. An increase in the thermal conductivity of the solid causes minimal delay in the solidification start times while accelerating the overall solidification period.

Future Work:

1. The most encouraging results with regard to the in-situ determination of thermal properties for molding sands were obtained by the method of Kirt et al [5]. Unlike the other methods examined, this method involves the gradual heating of the sand sample as opposed to a sudden temperature increase at one surface. Some of the difficulty, however, may be due to the fitting of the measured thermal profiles to an n th degree polynomial. Better results are expected if the thermal profiles in the sand are exactly described by a polynomial of known degree. Such conditions exist in the method proposed by Krischer [6] in which parabolic thermal profiles are created in a sand sample; end effects are eliminated by this method as well. Although this method is not an in situ method, it deserves a more detailed examination.
2. One source of difficulty was due to neglecting the fluid flow in the solidification code. A correct model of the fluid flow is necessary to more accurately model

the cooling of the melt as it flows through the rigging and mold cavity. This would immediately correct for the convective effects present in the casting and the non-uniform temperature distribution established in the mold and casting after the mold cavity is completely filled. These effects were not incorporated into the present code.

3. A second item is the model for the contact conductance. As discussed previously the model presently tested is highly simplified and does not treat the issues of stress and deformation during solidification. The contact conductance not only varies in time as stresses develop but is also influenced by the geometry of the mold cavity. The dissolved gas content in the melt can also significantly alter the behaviour at the contact. A more accurate contact model should improve results particularly for those cases where the thermal resistance of the gap at the casting/mold interface is large compared to that of the mold.
4. On a more general level, one problem often encountered in casting analysis is the large number of elements required to model the mold (possibly as high as 70% to 90% of the total elements). This can increase CPU time dramatically. It would be useful to employ a time varying effective heat transfer coefficient to represent both the mold and external environment.

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Appendix A

Further Detail on the Rappaz Model

The following is a more detailed description of the four phases of the Rappaz model (see chapter 3).

Phase 1: nucleation

Nucleation is a complex process requiring a critical amount of undercooling and proper inoculation conditions. Rappaz used a statistical approach in dealing with this first stage. He computed a continuous distribution to relate the nucleation rate to the undercooling. The integral of this distribution results in a relationship between grain density and undercooling. To simplify computations, the present code approximates this latter relationship with a cubic polynomial. During this first phase, the equiaxed grain is sufficiently small to render the release of latent heat from solidification negligible. The rate of enthalpy evolution simply becomes: $\dot{H} = C_p \dot{T}$ and the temperature can easily be computed. This stage continues until the nuclei density has reached its maximum, as indicated by the input parameters. The fraction of solid, f_s , during this stage is related to the nucleation rate, $\dot{n}$, and the grain radius, R :

$$f_s(t) = \int_0^t \dot{n}(\tau) \frac{4\pi}{3} R^3(\tau, t) d\tau$$

Phase 2: spherical growth

When the maximum nuclei density has been reached, the second phase of spherical growth begins. The grains in this stage are large enough to require inclusion of the latent heat contribution to enthalpy. The enthalpy formation is therefore: $\dot{H} = C_p \dot{T} + L \dot{f}_g$, where f_g describes the fraction of grain (see fig. 3.1). Since the

grain occupies a completely solid sphere, the fraction of solid (f_s) is equal to the fraction of grain. At the start, the internal fraction of solid, f_i , is one, this value drops below one at the onset of the third phase. During this stage the internal fraction of solid is related to the undercooling ahead of the solid/liquid interface (ΔT), the solute diffusion coefficient (D) and the velocity of the interface (v) by:

$$f_i = \Omega g(z) \quad (\text{A.1})$$

Here Ω represents the supersaturation of the liquid just ahead of the solid/liquid interface; this of course is indicative of the undercooling at the solidification front.

$$\Omega = \frac{C_L - C_o}{C_L - C_s}$$

with,

C_L	concentration of liquid ahead of interface
C_s	concentration of solid formed
C_o	initial/bulk concentration of the alloy

$g(z)$ is a factor which corrects for the solute layer around the grain envelope; it depends on the diffusivity, grain size and interface velocity. The fraction of solid (note: $f_s = f_i$) is related to the number of nuclei, n , the velocity of the advancing interface, v , and the grain radius, R_g . Implicit in R_g and v are the undercooling and solute diffusivity:

$$\dot{f}_g = 4\pi n v R_g^2$$

Based on Rappaz's work a system of differential equations was derived. Their simultaneous solution yields the fraction of solid as:

$$\dot{f}_s = 4\pi P(t)v(\Delta T)$$

The function $P(t)$ relates the nucleation rate and grain radius at each time step. $v(\Delta T)$ describes the velocity of the advancing solid/liquid interface as a function of undercooling, ΔT .

Figure A.1: Schematic of the solute diffusion model. (a) Three regions that can be distinguished: 1) solid dendrite, 2) interdendritic liquid where complete mixing of solute is assumed, and 3) liquid outside of the grain envelope where diffusion occurs. (b) and (c) Concentration profiles corresponding to (a). Source: [20].

Phase 3: dendritic growth

Solute and thermal balances are difficult to account for during the third phase since the solid within the grain envelope is no longer spherical, having developed dendritic arms. Figure A.1 describes the model during this stage. This model assumes a solute diffusion boundary layer, δ , ahead of the dendrite tips, with a linear solute distribution. Since $f_s \neq f_g$ and $f_i \leq 1.0$, both f_g and f_i must be accounted for. The enthalpy evolution becomes more complex:

$$\dot{H} = C_p \dot{T} - L \dot{f}_s = C_p \dot{T} - L (\dot{f}_i f_g + f_i \dot{f}_g)$$

Based on Rappaz's work, equations were derived to compute $\dot{f}_i$ and $\dot{f}_g$.

$$\dot{f}_g = 4 \pi n \left(\frac{3 f_g}{4 \pi n} \right)^{2/3} v$$

with:

n	nuclei density
v	velocity of dendrite tips

The internal fraction solid, f_i , is again computed from equation A.1.

Phase 4: impingement

The final phase of impingement occurs when f_g has grown to unity while f_i is still smaller than one. At this point the dendrite tips have reached the total radius, R_{tot} (see fig. 3.1). During this final phase, the governing differential equation is $div(k \nabla T) = (c_p \frac{dT}{dt} - L \frac{df_s}{dt})$. Since this phase is assumed to occur isothermally at the eutectic temperature (T_{eut}), $\frac{dT}{dt}$ is zero. During this phase, the relation between fraction of solid and enthalpy is simply expressed as:

$$-L\Delta f_s = \Delta H$$

At the start of the time step in this phase, upon reaching the eutectic, neither temperature (T_3) nor fraction solid (f_{s3}) at the end of the time step are known. To resolve this, an iterative approach is necessary whereby a first guess for the temperature results from the FEM thermal analysis; Δf_s is assumed to be zero at the start of the time step. From this we obtain a simple expression for the fraction of solid as:

$$-L\dot{f}_s = c_p \frac{T_3 - T_{eut}}{\Delta t}$$

Substitution into the FEM heat equation and subsequent iterations continue until convergence has reached acceptable tolerance levels. This phase continues until f_s reaches unity. At that point solidification is complete.

Appendix B

Derivation of the Full Expression for the Thermal Diffusivity

Following is the complete derivation for the expression of the thermal diffusivity shown in equation 2.3. The same nomenclature applies here as has been used throughout the text.

$$\rho C_p r \frac{\partial T}{\partial t} = \frac{\partial}{\partial r} \left(k r \frac{\partial T}{\partial r} \right) \quad (\text{B.1})$$

Assuming temperature dependence of the thermal conductivity, equation B.1 is expanded to:

$$\rho C_p r \frac{\partial T}{\partial t} = k \frac{\delta}{\delta r} \left(r \frac{\delta T}{\delta r} \right) + r \frac{\delta T}{\delta r} \frac{\delta k}{\delta T} \frac{\delta T}{\delta r}$$

or:

$$\frac{\delta T}{\delta t} = \frac{k}{\rho C_p r} \frac{\delta}{\delta r} \left(r \frac{\delta T}{\delta r} \right) + \frac{1}{\rho C_p} \frac{\delta k}{\delta T} \left(\frac{\delta T}{\delta r} \right)^2$$

Finally, the thermal diffusivity is solved for as:

$$\alpha = \frac{\frac{\delta T}{\delta t} - \frac{1}{\rho C_p} \frac{\delta k}{\delta T} \left(\frac{\delta T}{\delta r} \right)^2}{\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right)} \quad (\text{B.2})$$

The temperature dependent diffusivity, $\alpha(T)$, can then be evaluated at specified times and radial positions, t_i and r_i , as indicated in equation 2.3.

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