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Modelling Equiaxed Dendritic Solidification

by

Guojian Ma

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

Carleton University

Ottawa, Ontario

August 30, 1990

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The undersigned recommends to the Faculty of Graduate Studies and Research acceptance of the thesis: *Modelling Equiaxed Dendritic Solidification*, submitted by Guojian Ma, in partial fulfillment of the Degree of Master of Engineering.

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Abstract

An algorithm which was developed by Rappaz and Thevoz to describe the physics of equiaxed dendritic solidification is implemented in this thesis. This algorithm tracks the evolution of an equi-axed grain and predicts the transient and final microstructure for solidification. The grain evolves through four phases, i.e., nucleation, spherical growth, dendritic growth, and impingement. The fraction solid, fraction of inter-dendritic liquid and the grain size are computed. Coupling the solidification to the heat transfer analysis by using Rappaz' scheme and by using an iterative nonlinear solver are studied. For the nonlinear solver, different iterations, time steps, mesh sizes are tested and compared. The ordinary differential equations, which simulate the kinetics of grain growth, are solved by using an adaptive ordinary differential equation integration routine with automatic error checking.

An improved Rappaz' model for equi-axed dendritic solidification which was proposed by Dr. Hughes is also studied. An algorithm is implemented which describes the model and couples the solidification to the heat transfer.

Results from one dimensional test problems are listed and compared.

Dedication

To my Family

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List of Symbols

a_2	— — —	kinetic coefficient ($ms^{-1}k^{-2}$)
a_3	— — —	kinetic coefficient ($ms^{-1}k^{-3}$)
C_L	— — —	concentration in liquid (%)
C^*	— — —	concentration at interface (%)
C_s	— — —	concentration in solid (%)
C_o	— — —	initial concentration (%)
C_p	— — —	volumetric specific heat ($Jm^{-3}k^{-1}$)
D_s	— — —	diffusion coefficient in solid (m^2s^{-1})
f_g	— — —	fraction of grain
f_i	— — —	fraction of inter-dendritic liquid
f_L	— — —	fraction of liquid
f_s	— — —	fraction of solid
G	— — —	actual temperature gradient (km^{-1})
ΔG	— — —	change of total free energy
ΔG_v	— — —	change of volume free energy
$H, H(t)$	— — —	enthalpy
$\dot{H}, \dot{H}(t)$	— — —	enthalpy rate
k_o	— — —	partition coefficient
L	— — —	latent heat of fusion (Jm^{-3})
m_L	— — —	liquidus slope ($\%k^{-1}$)
n	— — —	grain density (m^{-3})
N_{max}	— — —	maximum grain density (m^{-3})
$\dot{n}$	— — —	grain density rate ($m^{-3}s^{-1}$)

N_i	---	basis function
p_e	---	peclet number
q	---	thermal flux
q_i	---	nodal thermal flux
r^*	---	critical radius
R_{tot}	---	radius of total grain (m)
R_g	---	radius of grain (m)
T	---	temperature ($^{\circ}C$)
T_{eut}	---	eutectic temperature ($^{\circ}C$)
T_L	---	liquidus temperature ($^{\circ}C$)
T_m	---	melting point ($^{\circ}C$)
T^*	---	temperature at interface ($^{\circ}C$)
ΔT	---	undercooling temperature ($^{\circ}C$)
ΔT_{max}	---	maximum undercooling ($^{\circ}C$)
t	---	time (s)
Δt	---	change in time (s)
v	---	velocity of grain growth (ms^{-1})
Θ	---	time weight
Ω	---	supersaturation
γ	---	surface free energy

Chapter 1

Introduction

In this chapter, we will briefly discuss the objective of the thesis and the layout of the thesis.

1.1 Objective of The Thesis

Solidification is a physical phenomenon that occurs during the material phase transformation from liquid into solid. It is particularly important in industrial processes such as casting and welding. Researches in solidification for both theory and mathematical models are of great importance to the whole study for the casting and welding processes. I. Minkoff believed that the two fields, solidification and crystal growth, enable an understanding and a description of cast microstructure [1].

Solidification in a metallurgical system is the process of transformation of a liquid material (of metal or alloy) to a solid. When a pure metal solidifies, growth of the solid phase involves the transfer of heat; while for an alloy, solidification involves both heat and the diffusion of the matter. The ideas common to solidification includes nucleation, dendritic growth, diffusion of the solute contents (for an alloy especially), heat flow, and growth kinetics.

This thesis is focused on equiaxed dendritic solidification. Much work has been

done in this field [9] [10] [11] [12] [13] [14] [15] [16] [17]. The goals of general solidification analysis are to calculate the temperature field and the distribution of solid within a casting or weld. For pure metals and eutectic alloys, numerical calculations of solidification usually assume that the latent heat is released at the equilibrium transformation temperature (melting point, T_m , for pure metal and eutectic temperature, T_{eut} , for eutectic alloys).

For non-eutectic alloys, microsegregation leads to the formation of a mushy zone within which the solid-liquid interface has a very complex shape. Latent heat release here is directly related to the evolution of the fraction of solid, f_s , within this two phase region. The basic theory of our equiaxed dendritic solidification comes from Rappaz and Thevoz [6], [7]. They made their model at a scale of one grain. The most significant characteristic of Rappaz and Thevoz's model is that they calculate the rejection and diffusion of solute, and thus relate the growth kinetics directly to the solute diffusion (i.e., kinetics are solute-controlled). Rappaz and Thevoz did not give a procedure for the whole development of the growth. They neglected spherical growth and the continuous evolution in the eutectic stage. Besides, Rappaz did not introduce iterations between the macroscopic calculation for temperature field and the microscopic calculations for the fraction of solid and the latent heat release. We experimented with an improved Rappaz's model that couples the solidification calculation to the heat equation, and introduces iterations between them. This model simultaneously calculates for both microscopic and macroscopic issues.

1.2 The Layout of The Thesis

This thesis is composed of seven chapters:

- Chapter 1 Introduction.

It is a brief prescription of the whole thesis.

- Chapter 2 Frontal Solidification

The frontal solidification theory is briefly discussed and three kinds of frontal solidification are listed and tested in the chapter. The three kinds of frontal solidification are:

- 1). Complete mixing of solute within the solid ($D_s = \infty$), which is called the Lever Rule.
- 2). No solute diffusion within the solid ($D_s = 0$), which is Scheil's model.
- 3). Partial solute diffusion within the solid (finite D_s value).

- Chapter 3 Solidification Theory

This chapter is focused on equiaxed dendritic solidification theory. Rappaz's model is discussed and the whole process of the grain growth is divided into four stages: Nucleation; Spherical growth; Dendritic growth; and Impingement eutectic. The evolution of the solidification in each stage is described and thus the mathematical model is established.

- Chapter 4 Algorithm and Numerical Methods

This chapter has two sections: One is focused on coupling solidification and the FEM heat equation. The method is briefly described in this chapter. The other is the discussion of ODEs and the code used to solve ODEs. LSODE program was used and some of its characteristics are discussed.

- Chapter 5 Results

In this chapter, the theory of equiaxed dendritic solidification is tested by comparison with Rappaz's example. The eutectic plateaus are also shown in our testing problems. Besides, we have coupled the solidification with

finite element analysis by using residual method and trying different iteration times. Different boundary conditions have also been tested. All the results are presented in the chapter.

- Chapter 6 Improved Rappaz' Mode

To couple solidification with the FEM heat equation, an improved Rappaz's model is presented in detail. This model, based on Rappaz's theory, is derived in a different way so that solving a system of ODEs with heat equation simultaneously enables us to introduce iterations between the macroscopic calculation and microscopic calculations. That makes the model more reasonable. Some test problems and results have also been presented in the chapter.

- Chapter 7 Conclusion and Future Work

Some conclusions are listed in the chapter and suggestions of future research work is also included in the chapter.

Chapter 2

Frontal Solidification

The controlled plane front solidification of an alloy is used in practice to grow single crystals, refine materials (e.g., zone refining), and obtain controlled uniform or non-uniform composition within the material growth [2]. Here, complete solute mixing is assumed. Complete solute mixing models are based on the assumption, when establishing a solute balance, that there is no local solute gradient within the liquid phase. Therefore, the local concentration within the liquid, C_L , is uniform and equals that concentration at the interface C_L^* . Under this assumption, and let D_s be the diffusion coefficient in the solid material, three different situations of solid state diffusion can be considered¹ :

- 1). Complete mixing of solute within the solid ($D_s = \infty$), which is called the Lever Rule;
- 2). No solute diffusion within the solid ($D_s = 0$), which is the Scheil's model;
- 3). Partial solute diffusion within the solid (finite D_s value).

¹Note: The main contents of section 1 to section 3 are come from M. Rappaz's paper, M. Rappaz's paper, MODELING OF MICROSTRUCTURE FORMATION IN SOLIDIFICATION PROCESS, see reference [8].

2.1 Solidification of Complete Solute Diffusion Within the Solid

Solidification with complete solute diffusion is also called *equilibrium solidification*. Solidification in crystal growth is almost never slow enough to approach equilibrium solidification.

Consider a liquid alloy of length L and initial composition C_0 freezing from one end. The first solid begins to form at T_L and is of composition kC_0 , lower in solute than the initial liquid composition. The balance of the solute is rejected from the solid-liquid interface and diffuses into the liquid, Fig. 2-1a. During subsequent cooling and solidification, both the liquid and solid become enriched in solute; at temperature T^* , the solid of composition C_s^* is forming in equilibrium at the solid-liquid interface with liquid of composition C_L^* .

Because diffusion in the solid and liquid is complete, the entire solid has uniform composition $C_s = C_s^*$ and the entire liquid of uniform composition $C_L = C_L^*$, Fig. 2-1b. At temperature T^* , a general materials balance is written:

$$C_s f_s + C_L f_L = C_0 \quad (2.1)$$

This is the *equilibrium lever rule*.

Consider the facts that:

$$f_L = 1 - f_s$$

$$C_L = (T_m - T^*)/m_L$$

$$C_s = C_L(1 - k) = (1 - k)(T_m - T^*)/m_L$$

$$C_0 = (T_m - T_L)/m_L$$

Figure 2.1: Solute redistribution in equilibrium solidification (copied from [2])

Change the lever rule into the form:

$$f_s = \frac{C_L - C_0}{C_L(1 - k)}$$

then we get:

$$f_s = \frac{1}{(1 - k)} \frac{T_L - T^*}{T_m - T^*} \quad (2.2)$$

$T_L - T^* = \Delta T$, so the fraction of solid f_s becomes a function of undercooling ΔT as below

$$f_s = \frac{1}{(1 - k)} \frac{\Delta T}{T_m - T^*} \quad (2.3)$$

The rate of solidification is

$$\dot{f}_s = \frac{-\dot{T}}{(1 - k)} \frac{T_m - T_L}{(T_m - T^*)^2} \quad (2.4)$$

From the equation 2.3, it is easy to see that the solid fraction is related mainly to the temperature field. The equation 2.4 shows that the rate of solidification depends primarily on the cooling rate, $\dot{T}$, for a given alloy.

The figure (2-2) shows the fraction of solid growth versus undercooling. For Al-7%Si alloy, the whole temperature range for solid fraction growth is 300°C . In reality, undercooling is unlikely to exceed several tens' degree of centigrade, where the eutectic temperature is encountered.

Figure 2.2: The Equilibrium planar solidification Diagram

Figure 2.3: Solute redistribution without solid diffusion (copied from [2])

2.2 Solidification without Diffusion in Solid

A case of more practical interest than the foregoing is the model without diffusion taking place at all in the solid. Consider the figure 2.3:

At the beginning the melt freezes at one end with a composition kC_0 . During the subsequent cooling and solidification, the liquid becomes richer in solute and so the solid that forms is of higher solute content at later stages of solidification. However, since there is no diffusion in the solid state, the

composition of the solid formed in the initial stages of freezing remains unchanged. At temperature T^* , solid of composition C_s^* is freezing from liquid of composition C_L^* and the solute distribution is shown as the figure 2.3. From the solute balance, we can get Scheil's model:

$$(c_L - c_s^*)df_s = (1 - f_s)dc_L \quad (2.5)$$

Substituting the equilibrium partition ratio, $k = C_s^*/C_L^*$, and integrating it from $c_s^* = kc_0$ at $f_s = 0$ yields the expression:

$$c_s^* = kc_0(1 - f_s)^{(k-1)}$$

Using the same analysis procedure, we get:

$$f_s = 1 - \left(\frac{T_m - T}{T_m - T_L} \right)^{\frac{1}{(k-1)}} \quad (2.6)$$

Fig.2-4, a test problem shows the relationship between the solid fraction growth and the temperature (here using undercooling).

Figure 2.4: Fraction Solid versus undercooling temperature for Scheil's model of solidification

2.3 Partial Diffusion in Solid

Between the extremes of the lever rule and Scheil's model, there is the case of partial diffusion in the solid. The general model of the planar solidification is expressed by Rappaz [8] as follows:

$$f_s = \frac{1}{1 - 2F'_{o,s}k} \left[1 - \left(\frac{T_m - T}{T_m - T_L} \right)^{\frac{(1 - 2F'_{o,s}k)}{k-1}} \right] \quad (2.7)$$

where:

$$F'_{o,s} = F_{o,s} [1 - e^{\frac{-1}{F_{o,s}}}] - \frac{1}{2} e^{\frac{-1}{2F_{o,s}}}$$

$F_{o,s}$ is the Fourier number for solid state diffusion, which is defined as:

$$F_{o,s} = \frac{D_s t_f}{x^2}$$

In which t_f is local solidification time(second); x_L is the length of element used in solute balance(m), $F_{o,s}$ is the Fourier number. When $F_{o,s} \rightarrow 0.0$, the expression becomes Scheil's model, when $F_{o,s} \rightarrow \infty$, the expression becomes the lever rule [8].

I have tried different $F'_{o,s}$ values, and from the results we can see the lever rule and the Scheil's models are really the two special conditions of the partial solute diffusion problems.

Figure 2.5: The partial diffusion model of solidification diagram.
Corresponds to equation 2.7, $F_{0,s} = 0.1$.

Figure 2.6: The partial diffusion model of solidification diagram.
Corresponds to equation 2.7, $F_{o,s} = 1.0$.

Figure 2.7: The partial diffusion model of solidification diagram
Corresponds to equation 2.7, $F_{0,s} = 10.0$.

Figure 2.8: Phase diagram and distribution of concentration before the interface (copied from [1])

2.4 Constitutional Supercooling

In metallic systems, growth of the solid from the liquid usually takes a cellular or a dendritic form. The two kinds of interfaces are forms of an instability characteristic of solidifying metals. This is the theory of 'constitutional supercooling' [1]. The constitutional supercooling theory relates to the unstable growth of a planar interface with undercooling due to the build-up of solute.

From the phase diagram in Fig.2.8 we can see the liquid changes in composition while freezing in the temperature range T_l to T_f . Because of the solute diffusion in the liquid, the solute rejected at the solid-liquid interface

builds up a boundary layer (Fig. 2.8(b))

The last liquid to solidify has the composition C_0/k_0 (see Fig. 2.8(a)). In growth, the boundary layer composition can increase to C_0/k_0 . At a certain distance far from the interface, the liquid composition again becomes C_0 (see Fig. 2.8(b)). The distribution of solute ahead of the interface is described as follows:

$$C_L = C_0 \left[1 + \left(\frac{1 - k_0}{k_0} \right) e^{-(Rx/D)} \right] \quad (2.8)$$

The liquidus temperature ahead of the solute boundary is given by the following expressing:

$$T = T_0 - mC_0 \left[1 + \left(\frac{1 - k_0}{k_0} \right) e^{-(Rx/D)} \right] \quad (2.9)$$

where R is the rate of advance of the solid interface or growth rate; x is the distance ahead of the interface; D is the diffusion coefficient in the liquid; m is the slope of the liquidus line; T_0 is the melting temperature of the pure metal; and k_0 is the equilibrium distribution coefficient [1].

If the actual temperature gradient is G , then the actual temperature ahead of the solid-liquid interface is:

$$T = T_i + Gx$$

where T_i is the actual temperature at the interface and is:

$$T_i = T_0 - m(C_0/k_0)$$

As G varies, a situation can arise where the liquid ahead of the interface is at a temperature below its equilibrium liquidus temperature, in this case a region of supercool liquid exists ahead of the interface.

Figure 2.9: Phase diagram and distribution of concentration before the interface (copied from [1])

This is shown in Figure 2.9(b) which shows the conversion of the graph relating composition ahead of the interface to temperature ahead of the interface. In Figure 2-9(b), the actual temperature gradient G is smaller than the gradient of the liquidus temperature T_{L_0} at the interface. For this condition, a point on the solid interface that grows ahead of the planar interface can still grow under conditions of greater supercooling. This means that any protuberance ahead of the interface will grow under favorable conditions.

A casting may show a structure that is totally columnar, totally equiaxed or a combination of the two. For an equiaxed solidification, the number of nuclei ahead of the interface is important².

²Note: This section mainly comes from I. Minkoff's book, Solidification and Cast Structure, see reference [1].

Chapter 3

Solidification Theory

This chapter is concerned with the existing theory of solidification for equiaxed dendritic growth alloys.

Figure 3.1 illustrates the basic ideas of equiaxed solidification. From the Figure we can see:

- f_g is the fraction of grain that is the ratio of the grain volume to the total volume at a certain time;
- f_s is the fraction of solid that is the ratio of the solid volume to the total volume;
- f_i is the fraction of the internal solid inside the grain which can be obtained from the ratio of the fraction of solid, f_s , to the fraction of grain, f_g .

The basic relations between them are as follows:

$$f_s = f_i f_g \quad (3.1)$$

$$\dot{f}_s = \dot{f}_i f_g + \dot{f}_g f_i \quad (3.2)$$

Equiaxed solidification involves several phenomena. First, nucleation occurs in an undercooled liquid. Secondly, when a nucleus appears, it grows spherically and inside the grain until it is all solid. When the radius of the grain

Figure 3.1: Basic concepts of equiaxed dendritic solidification

Figure 3.2: Four phases of grain growth: nucleation, spherical growth, dendritic growth, impingement

is larger than the critical radius [3] and if there is a constitutional super-cooled zone [1] [2] existing in front of the interface, then the growth becomes dendritic. The growth is controlled by the thermal and solute fields and by surface effects. Finally, when the grain grows large enough, say $R_g = R_{tot}$, the effects of the solute fields and the growth kinetic become very small and can be neglected. The thermal field then is the dominant factor controlling solidification. The solid inside a grain will impinge on the whole grain. Figure 3.2 shows the four stages of grain growth.

3.1 Macroscopic Model

In order to analyze the evolution of microstructure in a casting, we need to know the temperature field at the scale of the entire solidification process. The solidification process of alloys is primarily controlled by heat diffusion, so heat flow modeling is to be considered as below. Neglecting convection in the liquid zone, the temperature field can be described the energy equation:

$$\text{div}(k\nabla T) = C_p \frac{dT}{dt} - L \frac{df_s}{dt} \quad (3.3)$$

where:

- k is the thermal conductivity;
- C_p is the volumetric specific heat;
- L is the volumetric latent heat of fusion;
- T is temperature at a given point and is a function of space and time;
- f_s is the fraction of solid at a given point and is a more complicated function.

It should be noted that in the above equation, all the thermal physical properties of the materials, k and C_p in particular, may be temperature and space dependent.

From the heat flow equation, there exists two fields: temperature field and f_s . So an additional equation is needed. That is the task of the microstructure model and will be presented in the succeeding sections in which the equiaxed dendritic solidification will be discussed in detail and the development of the fraction of solid, $f_s(T, \dot{T}, n, \dots)$, will be deduced.

There are two methods in numerical solutions for the heat flow equation for solidification

1. Equivalent specific heat method:

$$\frac{df_s}{dt} = \frac{df_s}{dT} \frac{dT}{dt} = \frac{df_s}{dT} \dot{T}$$

the heat flow equation then becomes :

$$\text{div}(k\nabla T) = (C_p - L \frac{df_s}{dT}) \dot{T}$$

let $C_p^e(T) = (C_p - L \frac{df_s}{dT})$ to be the equivalent specific heat, the heat equation finally becomes:

$$\text{div}(k\nabla T) = C_p^e(T) \dot{T} \quad (3.4)$$

2. The enthalpy method

we have:

$$H(T) = \int_0^T C_p(T_x) dT_x + L(1 - f_s(T))$$

the heat flow equation becomes:

$$\text{div}(k\nabla T) = \dot{H}(T) \quad (3.5)$$

Rappaz indicated that the equivalent specific heat and temperature curve exhibits a discontinuity at the melting point for pure metal (or eutectic temperature for eutectic alloys) and the method can not conserve energy. On the other hand, however, using enthalpy method can avoid these disadvantages [8]. So we have used the enthalpy method.

3.2 Nucleation

3.2.1 Nucleation Distribution

The heterogeneous nucleation theory outlined by Turnbull and Fisher [8] is believed to be inadequate for reproducing experimental results and does not

reflect the complex nucleation phenomena in real alloys. Furthermore, the basic mechanisms of inoculation are not yet completely understood. Rappaz (et al), taking a statistical approach to solve the nucleation distribution problem, have assumed that quasi-instantaneous nucleation occurs on a set of nucleation sites that is characterized by a continuous distribution (Gaussian distribution, for example) rather than a discrete distribution, $dn/d(\Delta T)$ (see figure 3.3). At a given undercooling ΔT , the grain density is given by the integral of the distribution. Therefore, given three parameters of the distribution, for example, mean nucleation undercooling, ΔT_N ; standard deviation of the distribution, ΔT_σ ; and maximum density of nuclei, N_{max} , we can calculate the grain density corresponding to the undercooling by integration. These adjustable nucleation parameters can be deduced easily from experiments [9].

From the figure, we can see that at a given undercooling, ΔT_1 , the grain density is given by the integral of the nucleation site distribution from zero to ΔT_1 , e.g. N_1 in figure 3.3 corresponding to ΔT_1 . By this means, the grain density is updated at each time step as a function of undercooling [9].

Rappaz's distribution of nucleation is easier to apply in engineering, but to save the time of the integral of the distribution of nucleation in computing the grain density, n , we use a polynomial as the function of undercooling, ΔT , to calculate the value of grain density. For example:

$$n = \int_{\Delta T_1}^{\Delta T_2} n d\Delta T \approx P(\Delta T)$$

$P(\Delta T)$ has the following cubic polynomial form:

$$n = N_{max} \left(\frac{\Delta T_{max}}{\Delta T_{nmax}} \right)^2 \left(3 - 2 \frac{\Delta T_{max}}{\Delta T_{nmax}} \right) \quad (3.6)$$

Where, N_{max} is the maximum density of nuclei; ΔT_{nmax} is the maximum undercooling at which all nuclei become active; ΔT_{max} is the maximum

Figure 3.3: Continuous distribution of nucleation sites used in modelling of equiaxed solidification. Copied from Rappaz' paper [9].

Figure 3.4: Comparison of the results of grain density from a). cubic polynomial, and b). Gaussian distribution

undercooling that has ever appeared up to the current time.

The result of this approximation is shown in Figure 3.4 compared with the result from the integral of Gaussian distribution.

From the results presented above, we can easily see that the approximation is very near the integral of Rappaz's statical nucleation distribution and it is simpler to calculate.

3.2.2 Nuclei Grain Growth

On nucleation, the equiaxed grain is spherical. The radius is sufficiently small so that the rate of release of latent heat from solidification can be neglected. Thus the enthalpy rate equals the temperature rate times volumetric heat capacity:

$$\dot{H} = C_p \dot{T} - L \dot{f}_s = C_p \dot{T} \quad (3.7)$$

It is assumed that there is no liquid inside the grain, i.e., $f_l = 1.0$. The fraction of grain is considered less than 10^{-4} to 10^{-3} .

The problem is to compute the $\frac{\text{volume solid}}{\text{unit volume}}$. This is the fraction solid of the average grain.

The conditions are: $f_i = 1.0$, $0.0 \leq f_g < 1.0 * 10^{-3}$.

The fraction of solid $f_s(t)$ is the sum of the contributions of all of the grains, which have been nucleated at a time τ smaller than t which have grown between τ and t . Thus, the $f_s(t)$ can be written as:

$$f_s(t) = \int_0^t \dot{n}(\tau) \frac{4}{3} \pi R^3(\tau, t) d\tau \quad (3.8)$$

Where $\dot{n}(\tau)$ is the nucleation rate at time τ and $R(\tau, t)$ is the radius of the grains which have been nucleated then and have grown until time t . Differentiating equation 3.8 gives:

$$\frac{df_s(t)}{dt} = \dot{n}(t) \frac{4}{3} \pi R^3(t, t) + \int_0^t \dot{n}(\tau) 4\pi R^2(\tau, t) \frac{\partial R(\tau, t)}{\partial t} d\tau$$

The first term on the right hand side of the equation is associated with the nucleation of new grains. It can be neglected. On the other hand, the velocity of the grain interface at time t , $v(\tau, t) = \frac{\partial R(\tau, t)}{\partial t}$, is a function only of the undercooling $\Delta T(t)$ of the grains interface. One can then, as Rappaz

has suggested [long], write:

$$\frac{df_r(t)}{dt} = \int_0^t \dot{n}(\tau) 4\pi R^2(\tau, t) v(\tau) d\tau \quad (3.9)$$

Considering the following facts:

$$\begin{aligned} \dot{n}(t) &= \frac{dn(t)}{dt} = \frac{dn}{d\Delta T} \frac{d\Delta T}{dt} \\ \frac{dn}{d\Delta T} &= 6 \frac{\Delta T_{maz}}{(\Delta T_{nmaz})^2} \left(1 - \frac{\Delta T_{maz}}{\Delta T_{nmaz}} \right) N_{maz} \end{aligned}$$

Here $\Delta T_{maz} = \Delta T(\tau)$ when τ is small enough so solidification is still in the stage before the recalescence. We have:

$$\frac{dn}{d\Delta T} = 6 \frac{\Delta T(\tau)}{(\Delta T_{nmaz})^2} \left(1 - \frac{\Delta T(\tau)}{\Delta T_{nmaz}} \right) N_{maz} \quad (3.10)$$

Because in a short period, the relationship between $\Delta T(\tau)$ and $\dot{T}$ is as follows:

$$\frac{d\Delta T(\tau)}{d\tau} = \frac{d(T_L - T)}{d\tau} = -\dot{T}$$

which leads to:

$$d\tau = \frac{d\Delta T}{-\dot{T}}$$

So:

$$\begin{aligned} \dot{n}(t) &= \frac{6N_{maz}}{\Delta T_{nmaz}^2} \left(\Delta T \frac{d\Delta T}{dt} - \frac{\Delta T^2}{\Delta T_{nmaz}} \frac{d\Delta T}{dt} \right) \\ &= \frac{6N_{maz}}{\Delta T_{nmaz}^2} \left(\dot{T}^2 t + \frac{\dot{T}^3}{\Delta T_{nmaz}} t^2 \right) \\ &= \frac{6N_{maz}\dot{T}^2}{\Delta T_{nmaz}^2} \left(t + \frac{\dot{T}}{\Delta T_{nmaz}} t^2 \right) \end{aligned} \quad (3.11)$$

$$\begin{aligned} R(\tau, t) &= \int_{\tau}^t v(\Delta T(s)) ds \\ &= \int_{\tau}^t a_2 (\Delta T(s))^2 ds \\ &= \int_{\tau}^t a_2 (-\dot{T}s)^2 ds \\ &= \frac{a_2 \dot{T}^2}{3} (t^3 - \tau^3) \end{aligned} \quad (3.12)$$

By bring these two expressions into integration for expressing fraction of solid and assuming $\dot{T}$ is constant during one FEM time step, eq. 3.8 and 3.9 become:

$$f_s = \int_0^t \dot{n}(\tau) \frac{4\pi}{3} R^3(\tau, t) d\tau \quad (3.13)$$

$$\dot{f}_s = \int_0^t \dot{n}(\tau) 4\pi R^2(\tau, t) v(\tau) d\tau \quad (3.14)$$

Using LSODE to solve f_s from $\dot{f}_s$.

3.3 Critical Radius

The formation of one phase by the aggregation of components of another phase without change of composition and without being influenced by impurities or external surface is called homogeneous nucleation. In most engineering casting, heterogeneous nucleation theory is applied, in which impurity particles and external surfaces are taken into account [3].

If a spherical embryo of solid is formed within a uniform liquid, the free energy changes. This is associated with two different free energy items:

- The change of volume free energy of the atoms in the solid and liquid, ΔG_v ;
- The surface free energy of the embryo, γ .

For a spherical embryo of radius r , the overall change in free energy, ΔG , is given by:

$$\Delta G = 4\pi r^2 \gamma + \frac{4}{3}\pi r^3 \Delta G_v \quad (3.15)$$

Figure 3.5: The change of free energy resulting from the formation of a spherical embryo of solid in the liquid

where γ is the surface energy (erg cm^{-2}), ΔG_v is the volume free energy change (erg cm^{-3}). Above the melting point, T_m , ΔG_v is positive and below it ΔG_v is negative. Fig.3.5 shows the variation of the different free energy terms below T_m and the overall change in free energy. Any embryos which form above T_m will rapidly disperse. On the other hand, below T_m , provided the embryo reaches a critical size with radius r^* , at which:

$$\left(\frac{\partial(\Delta G_v)}{\partial r}\right) = 0 \quad (3.16)$$

it is equally probable that the embryo will disperse or that it will grow as a stable nucleus. Differentiating the equation of change in free energy we find:

$$r^* = \frac{2\gamma}{\Delta G_v} \quad (3.17)$$

considering:

$$\Delta G_v = L_m \left(1 - \frac{T}{T_m}\right) = \frac{L_m \Delta T}{T_m}$$

Where ΔT is undercooling; L_m is the latent heat of melting; T_m is the temperature at melting point. We finally get:

$$r^* = \frac{2\gamma T_m}{L_m \Delta T} \quad (3.18)$$

This is the expression of critical radius r^* related to the undercoolings.

Since ΔG_v increases approximately linearly as the temperature falls, the critical radius decreases rapidly as the undercooling increases.

For heterogeneous nucleation, most nucleation phenomena in liquids take place at an undercooling significantly less than that predicted by theories of homogeneous nucleation (a few degrees below the melting point compared with several hundreds of degrees below the melting point).

Figure 3.6: The change of free energy corresponding to the undercooling temperature

The expression of critical radius is much like that of homogeneous nucleation. For example, the critical radius for heterogeneous nucleation of the cap-shaped model is:

$$r^* = \frac{2 \alpha \gamma_\beta}{\Delta G_v} \quad (3.19)$$

where $\alpha \gamma_\beta$ is the interfacial energy between α and β phases [1], [2].

3.4 Spherical Growth

In solidification with spherical growth, the equiaxed grain is still spherical, but it has grown large enough so that the release of latent heat is significant. Thus the enthalpy rate should also consider the latent heat release by solidification, i.e.:

$$\dot{H} = c_p \dot{T} + L \dot{f}_g \quad (3.20)$$

The condition is: $f_i = 1.0$

We have:

$$v = a_2 \Delta T^2 + a_3 \Delta T^3$$

Or as Rappaz [9] suggested, the velocity of dendrite tip growth is related to the solute undercooling by:

$$\frac{dR_g}{dt} = \frac{D}{\pi^2 \Gamma m C_0 (k-1)} (T^* - T_\infty)^2$$

Where Γ is the Gibbs-Thomson coefficient and T_∞ is the temperature far ahead of the tip. Rappaz thought T_∞ could be associated with the concentration, C_R , at the radius $r = R_{tot}$. Consequently he gave another expression for velocity of dendrite tip growth:

$$\frac{dR_g}{dt} = \frac{D m C_0}{\pi^2 \Gamma (k-1)} \left(\frac{C^* - C_R}{C_0} \right)$$

which is exactly the form:

$$\begin{aligned} \frac{dR_g}{dt} &= \frac{D}{\pi^2 \Gamma (k-1) m C_0} (m(C^* - C_R))^2 \\ &= a_2 (m(C_0 - C_R))^2 \end{aligned} \quad (3.21)$$

Here $a_2 = \frac{D}{\pi^2 \Gamma (k-1) m C_0}$:

$$\begin{aligned} R_g &= \int_0^t v(t) dt \\ &= \left(\frac{3 f_g}{4 \pi n} \right)^{\frac{1}{3}} \end{aligned} \quad (3.22)$$

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

using LSODE we can calculate f_g from this $\dot{f}_g$. Then:

$$\dot{T} = \frac{\dot{H} + L\dot{f}_g}{cp} \quad (3.23)$$

$\dot{T}$ is not a constant at this stage.

To calculate the value of f_i we have:

$$f_i = \Omega g(z) \quad (3.24)$$

where:

$$\begin{aligned} \Omega &= \frac{C_L - C_0}{C_L - C_s} \\ &= \frac{C_L - C_0}{C_L(1 - k)} \\ &= \frac{\Delta T}{(\Delta T + mC_0)(1 - k)} \end{aligned} \quad (3.25)$$

and

$$g(z) = 1 + 1.5z + z^2 + 0.25z^3 \quad (3.26)$$

where:

$$z = \frac{2D}{vR_g} = \frac{1}{P_e}$$

D is the diffusion coefficient; v is the velocity of dendrite tip growth.

$$f_s = f_g \quad (3.27)$$

At the beginning of the calculation, this value of f_i is larger than 1.0. This is meaningless and so it is assigned a value of unity. At a certain time the value of f_i drops below the unity. This indicates the start of dendritic growth which we call phase 3.

3.5 An Algorithm for Phase 1 & Phase 2

In real castings, the time for phase 1, nucleation stage, and phase 2, spherical growth, is very short and their influences on the latent heat release are not too large. We follow Dr. Hughes in deriving a system of differential equations to describe the development of solidification in these two stages. We know that the dendrite tip grows with a velocity $v(\Delta T)$ or $v(c^*)$ and the grain density distribution $\dot{n}$:

$$\dot{n} = 6N_{max} \frac{\Delta T_{max}}{(\Delta T_{nmax})^2} \left(1 - \frac{\Delta T_{max}}{\Delta T_{nmax}}\right)$$

let $f(x) = \dot{n}$

$$\begin{aligned} n(t) - n(0) &= \int_0^t f(\Delta T(s)) \Delta \dot{T}(s) ds \\ &= \int_{\Delta T(0)}^{\Delta T(t)} f(z) dz \\ &= F(\Delta T(t)) - F(\Delta T(0)) \end{aligned} \quad (3.28)$$

Where F is a primitive of f . So $n(t) - n(0)$ is a *known* function of ΔT , say:

$$n(\tau) - n(0) = \Phi(\Delta T(t))$$

from the sections mentioned before, we have:

$$\begin{aligned} \dot{f}_s &= \int_0^t \dot{n}(\tau) 4\pi R^2(\tau, t) v(\tau) d\tau \\ &= 4\pi P(t) v(\Delta T(t)) \end{aligned} \quad (3.29)$$

where:

$$P(t) = \int_0^t \dot{n}(\tau) R^2(\tau, t) d\tau$$

and similarly:

$$\dot{P}(t) = 2Q(t) v(\Delta T(t))$$

where:

$$Q(t) = \int_0^t \dot{n}(\tau) R(\tau, t) d\tau$$

and finally:

$$\dot{Q}(t) = v(\Delta T(t)) \int_0^t \dot{n}(\tau) d\tau = (n(t) - n(0))v(\Delta T(t)) = \Phi(\Delta T(t))v(\Delta T(t))$$

Thus it leads to a system of ordinary differential equations(ODEs):

$$\begin{aligned}\dot{Q} &= \Phi(\Delta T)v(\Delta T) \\ \dot{P} &= 2Qv(\Delta T) \\ \dot{f}_s &= 4\pi P(t)v(\Delta T)\end{aligned}\tag{3.30}$$

with initial conditions $Q(0) = P(0) = f_s(0) = 0$. $\dot{R}_g = v(\Delta T)$.

To solve this we need to know $\Delta T = T_L - T$ over the interval $[0, t]$.

(Again, note that Q , P and f_s are defined at each point $x \in \Omega$, i.e., $f_s = f_s(x, t)$, $P = P(x, t)$, $Q = Q(x, t)$. There is a separate system (1.29) at each x , and they are all independent. (i.e., the system (1.29) for x_1 is independent of the systems (1.29) for $x_2 \neq x_1$. This is in contrast to the functions defined by partial differential equations in which there would be coupling between the systems (1.29) at different values of x).

3.6 Dendritic Growth

3.6.1 Theory of Dendritic Grain Growth

During dendritic grain growth, the equiaxed grain is no longer spherical because the dendrites have started to form. The ratio of solid volume inside the grain to the volume of grain, f_i , which was unity just after the nucleation (in the nucleation and spherical growth stages), decreases rapidly as

Figure 3.7: Schematic representation of equiaxed dendritic solidification

the dendritic grain develops, and then returns to unity again at the end of solidification. Because the thermal diffusivity of metallic alloys is 3-4 orders of magnitude greater than the solute diffusivity, the kinetics of dendrite tip is solute controlled [6] [7].

M. Rappaz and Ph. Thévoz developed a model for equiaxed dendritic grain growth [6] [7]. This model is summarised in Figure 3.6 and they proposed some hypotheses:

1. rapid thermal diffusion within the scale of the grain. Accordingly, the temperature is uniform and the dendrite interface is an isoconcentration surface;
2. complete solute mixing is assumed within the interdendritic liquid;

3. spherical solute diffusion outside the grain envelope (region 3);
4. no back-diffusion of solute within the solid;
5. solute conservation within the whole volume of radius, R_{tot} ;
6. thermal balance is satisfied; and
7. a quadratic kinetics law relates the speed of a dendrite tip, v , to the undercooling.

They divided the whole region into three. Region 1 is solid; region 2 is liquidus inside the grain; and region 3 is liquidus outside the grain [6]. In their later paper [7], they further used a solute layer with thickness of δ to replace the solute diffusion [7]. Upon the above hypotheses and the solute layer, they set up a mathematical model or the solute balance which finally gives:

$$\delta = \frac{2D}{v} \quad (3.31)$$

where D is the diffusion coefficient and v is the velocity of dendrite tip growth.

According to the hypothesis 5, solute conservation within the whole volume of R_{tot} , they set the relationship between the fraction of solid, f_s , the fraction of grain, f_g , and the fraction of internal solid, f_i , as:

$$f_i = \frac{f_s}{f_g} = \Omega g(z) \quad (3.32)$$

in which:

$$g(z) = 1 + 1.5z + z^2 + 0.25z^3 \quad (3.33)$$

and:

$$z = \frac{\delta}{R_g} = \frac{2D}{R_g v} = \frac{1}{Pe}$$

where R_g is the radius of grain; and Pe is the Péclet number of the spherical grain. In equation (3.32) Ω is supersaturation. This model works well a long

as the solute layer with thickness, δ , has not reached the limit, R_{tot} , within which the grain is allowed to grow. When the solute layer reaches the limit, R_{tot} , the solute concentration, C_R , at $r = R_{tot}$ is increased to conserve the solute. As the solute concentration C_R increases, the velocity of dendrite tip growth which in fact is related to the concentration¹ slows down till almost complete mixing of solute is reached. When the interface concentration, C^* , reaches the eutectic value, C_{eut} , grain growth is ended (i.e., $f_g \approx 1.0$) and any nucleation or kinetics of eutectic grain growth is neglected. Then the final stage, the impingement of solid to the grain boundary, starts. In that stage, the solidification is assumed to be isothermal.

3.6.2 An Algorithm for Dendritic Grain Growth

In this stage the solid fraction, f_s , is no longer equal to the grain fraction, f_g (i.e. $f_i \leq 1.0$). the solidification rate has contributions from both f_g and f_i . Thus the enthalpy rate becomes:

$$\dot{H} = cp\dot{T} - L\dot{f}_s = cp\dot{T} - L(\dot{f}_i f_g + f_i \dot{f}_g) \quad (3.35)$$

¹from spherical growth we know that:

$$\begin{aligned} \frac{dR_g}{dt} &= \frac{D}{\pi^2 \Gamma(k-1)} (T^* - T_\infty)^2 \\ &= \frac{DmC_0}{\pi^2 \Gamma(k-1)} \left(\frac{C^* - C_R}{C_0} \right)^2 \\ &= a_2 (m(C^* - C_R))^2 \end{aligned} \quad (3.34)$$

here $a_2 = \frac{D}{mC_0 \pi^2 \Gamma(k-1)}$.

The fraction of grain is considered less than 1.0, i.e., $f_g < 1.0$.

$$R_{tot} = \left(\frac{3}{4\pi n} \right)^{\frac{1}{3}} \quad (3.36)$$

$$v = a_2(m(c_* - c_R))^2 \quad (3.37)$$

where m is the slope of the liquidus line.

$$R_g = R_g(t_1) + \int_{t_1}^{t_2} v(t) dt = \left(\frac{3f_g}{4\pi n} \right)^{\frac{1}{3}} \quad (3.38)$$

$$f_g = 4\pi n R_g^3 v \quad (3.39)$$

$$f_g = \int_0^t \dot{f}_g dt \quad (3.40)$$

$$\delta = \frac{2D}{v} \quad (3.41)$$

$$\Omega = \frac{c_* - c_0}{c^*(1-k)} = \frac{c_* - c_0}{c_0(1-k)} \quad (3.42)$$

$$g(z) = (1 + 1.5z + z^2 + 0.25z) \quad (3.43)$$

where $z = \frac{2D}{R_g v}$

$$\dot{f}_g = \dot{\Omega} g(z) = \frac{g(z) \dot{c}^*}{c_0(1-k)} = \frac{g(z) \dot{T}}{m c_0(1-k)} \quad (3.44)$$

$$\dot{\Omega} = \frac{\dot{H} + L f_g \dot{f}_g}{C_p k \Delta T_0 - L g(z) f_g} \quad (3.45)$$

$$\dot{T} = k \Delta T_0 \dot{\Omega} \quad (3.46)$$

When $\delta + R_g \geq R_{tot}$, we increase the solute concentration c_R at R_{tot} conserve solute and thus change the value of both v and Ω .²

²At this time, when $\delta + R_g \geq R_{tot}$ the real value is no longer $\delta = \frac{2D}{v}$, the solute conservation is within the total volume, so we use equivalent diffusion layer δ^* to instead δ .

$$\delta^* = R_{tot} - R_g$$

When f_g grows to unity but f_s is still smaller than unity, phase 4 starts.

We have used solute conservation to increase the value of c_R , it gives a reasonable result (see Fig. 3.7). We also have tried neglecting the solute layer thickness δ in the final stage in dendritic grain growth (see Fig. 3.8 and 3.9). From the two results, it is easy to see that increasing the value of c_R has great influence on the grain growth. It makes the speed of the growth curve of f_g slow down.

Figure 3.8: Solidification curve with solute concentration c_R at R_{tot} increasing.
a). Temperature curve b). Fractions of solid and grain

Figure 3.9: Solidification curve without solute concentration c_R at R_{tot} increasing
a). Temperature curve. b). Fraction of solid and grain (solid curve is fraction of grain, dashed curve is fraction of solid)

3.7 Impingement

Impingement is reached when solid dendrite tips impinge onto the liquid grain envelop. In this stage, because $f_g = 1.0$, the radius of grain, R_g , has reached the value of total radius, R_{tot} . Thus kinetics of grain growth are neglected. The solidification is assumed to be isothermal, that means dT^*/dt is negligible. The only thing related to the solidification is the heat balance. From section (3-1) heat flow equation and the condition in this particular phase, we have:

$$\begin{aligned} \text{div}(k\nabla T) &= C_p \frac{dT}{dt} - L \frac{df_s}{dt} \\ \dot{f}_s &= C_{fs}(T_{eut} - T)^2 \end{aligned} \quad (3.47)$$

where:

$$C_{fs} = \frac{f_s}{\Delta t} \left(\frac{1}{\Delta T_{eut}} \right)^2 \quad (3.48)$$

Here, T_{eut} is eutectic temperature; ΔT_{eut} is the undercooling below the eutectic temperature. In case of $\dot{f}_s$ becomes too large, we have to give a restriction so that the growth of f_s will not be allowed to exceed 1.0.

$$\dot{f}_s = \frac{1 - f_s}{\Delta t}$$

Then the value of $\dot{f}_s$ will be:

$$\dot{f}_s = \min\{C_{fs}(T_{eut} - T)^2, \frac{1 - f_s}{\Delta t}\}$$

With $\dot{f}_s$ solved, we have:

$$f_s = f_s(t_1) + \int_{t_1}^{t_2} \dot{f}_s dt \quad (3.49)$$

As to the fraction of internal solid, f_i , we have:

$$f_i = \frac{f_s}{f_g} = f_s \quad (3.50)$$

When f_s grows to 1.0, f_i increase to unity too, and the solidification process stops.

It might happen that the impingement starts with $T > T_{eut}$, under this circumstance we simply assume $\dot{T} = 0$, the solidification rate, $\dot{f}_s$, then directly related to the heat flux.

Chapter 4

Algorithm and Numerical Methods

An important use of the microstructure of solidification is to couple the microstructure to the macro-calculation of the temperature field of the whole casting process. In this chapter, the algorithm and numerical methods will be presented briefly and the use of ODE solvers including LSODE will also be discussed.

4.1 Coupling Microstructure of Solidification to Continuum Mechanics

Basic Equations for Heat Transfer

The conservation of energy for conductive heat transfer including latent heat is:

$$H(T) = \int_{T_{ref}}^T C_p dT + L(1 - f_s) \quad (4.1)$$

Where $H(T)$ is enthalpy; C_p is volumetric heat; L is latent heat; and f_s is the fraction of solid in the melt. Thus the heat diffusion equation becomes:

$$\text{div}[k \nabla T(x, t)] = C_p \dot{T} + L \dot{f}_s + Q \quad (4.2)$$

Here k is the thermal conductivity.

In the finite element analysis, we have the following expression

$$CT - L\dot{f}_s + KT + Q = 0 \quad (4.3)$$

Here K is the conductivity matrix; C , L are capacitance and latent heat matrixes. This is a set of nonlinear ODEs.

Equation for Solidification

The fraction of solid in the melt for equiaxed dendritic solidification has the relationship:

$$f_s = f_i f_g \quad (4.4)$$

Where f_g is fraction of grain; and f_i is the internal fraction of solid.

$$\dot{f}_s = \dot{f}_i f_g + \dot{f}_g f_i \quad (4.5)$$

4.1.1 Nonlinear Solution

For heat transfer problems, the actual solution for transient problems was generally difficult and indeed not available for non-linear situations. Therefore, the following method is used to solve the problem.

1. Residual Method Used in Heat Transfer Problem

At any time step t_i , suppose T_1 , T_3 , f_{s1} , f_{s3} are known, where T_1 and T_3 are the temperatures; and f_{s1} and f_{s3} are the fractions of solid at the start of the time step and at the end of the time step respectively. The heat diffusion equation, eq.4.3, then becomes:

$$C \left(\frac{T_3 - T_1}{\Delta t} \right) - L \left(\frac{f_{s3} - f_{s1}}{\Delta t} \right) + K[\theta T_3 + (1 - \theta)T_1] + Q = 0 \quad (4.6)$$

The equation should be satisfied if Δt is small enough. If the real solution T_3 at time step t_i is not known, we first give a value of T_3 , say T'_3 . Then there exists a ΔT_3 such that

$$T'_3 + \Delta T_3 = T_3 \quad (4.7)$$

Substitute (4.7) into (4.6), to get:

$$\frac{C}{\Delta t}(T'_3 + \Delta T_3 - T_1) - \frac{L}{\Delta t}(f_{s3} - f_{s1}) + K[\theta(T'_3 + \Delta T_3) + (1-\theta)T_1] + Q = 0 \quad (4.8)$$

$$\left(\frac{C}{\Delta t} + K\theta\right) \Delta T_3 = -\frac{C}{\Delta t}(T'_3 - T_1) + \frac{L}{\Delta t}(f_{s3} - f_{s1}) - K[\theta T'_3 + (1-\theta)T_1] - Q \quad (4.9)$$

The right side of equation (4.9) is called the residual.

so:

$$\left(\frac{C}{\Delta t} + K\theta\right) \Delta T_3 = \text{Residual} \quad (4.10)$$

Using the following iterative sequence:

$$T_3^{i+1} = T'_3 + \Delta T_3^i \quad (4.11)$$

$$\dot{H}^{i+1} = \frac{C}{\Delta t}(T_3^{i+1} - T_1) - \frac{L}{\Delta t}(f_{s3}^i - f_{s1}) \quad (4.12)$$

Then, the solidification code is used with these values of $\dot{H}^{i+1}$ and T_3^{i+1} , to obtain f_{s3}^{i+1} . Again, we use the residual equation

$$\left(\frac{C}{\Delta t} + K\theta\right) \Delta T_3^k = -\frac{C}{\Delta t}(T_3^{k-1} - T_1) + \frac{L}{\Delta t}(f_{s3}^{k-1} - f_{s1}) - K[\theta T_3^{k-1} + (1-\theta)T_1] - Q \quad (4.13)$$

After several iterations, the energy equation might converge to a certain tolerance.

2. Distribution of Nodal Loads to the Gauss Points

Because the heat diffusion equation is evaluated at Gauss points and more information can be obtained from Gauss points, it is

necessary to interpolate the nodal loads (such as temperature, flux, etc.) to the Gauss points using the basis function (N matrix).

$$T_s^{gn} = \sum_i^{nodes} N_i T_i^{nn}$$

4.2 Discussion of the ODEs

In the algorithm for equiaxed dendritic solidification in this thesis, there are three ordinary differential equations that represent the development of grain growth, fraction of solid, and the temperature field. To integrate these ordinary differential equations, an ODE solver has been adopted in the present work. This ODE solver has been developed after years of research at Lawrence Livermore National Laboratory [18]. This solver can be used with large time steps for solving ODEs. In the analysis of the four phases of growth, to reflect the features of f_g , f_s , and temperature, particularly in phase 2 and phase 3 (spherical growth and dendritic growth) we have adopted small time steps (such as 0.4 seconds) in the microstructure and in phase 4 (impingement) we have used large time steps (such as 1.0, 2.0, 5.0 seconds) in the microstructure. In coupling latent heat to FEM heat transfer problems, because of the Residual method used, the finer time steps have been adopted. This solver automatically checks the error in each time step. It subdivides the time step into smaller time steps if necessary, according to the acceptable tolerance of error. The use of this solver has made the solidification code efficient and it predicts accurate results as shown in the previous chapter.

To solve the ordinary differential equations, we tried the simple Euler method,

which typically have the form:

$$Y_n = Y_{n-1} + h_n f(t_{n-1}, Y_{n-1})$$

where $h_n = t_n - t_{n-1}$ is the size of the time step. The major problem of applying the Euler method to solve ODE is that the explicit method defines the new value directly from the known previous values and the next solution point is computed at time $t_n = t_{n-1} + h_n$ by moving from the point (t_{n-1}, y_{n-1}) on a line at a constant slope of $f(t_{n-1}, y_{n-1})$, here $f(t, y) = dy/dt$. That method not only produces an error in the solution but also needs very small time steps. Figure (5.1) shows schematically how this error is measured as an amount by which the true solution to the ODE differs from the numerical solution.

Because of the problems mentioned above, the simple Euler method didn't work well. The present work is done by using an ODE solver from LLNL [18]. Paramjeet Khorai [21] has compared different ODE solvers and he suggested using the ODE solver developed by LLNL. LLNL has developed many solvers. Among them the LSODE is the "standard choice" for ODE initial-value problems [18]. In the LSODE there are four parameters which should be specified for accurate solution of the problem. These parameters are

- non-stiffness or stiffness of equation
- tolerance for error calculations
- time step
- starting value of phase fraction

All the ODE equations in my work are non-stiff. This is confirmed by Fig. 4.2. This figure shows families of curves with different initial values of func-

Figure 4.1: Error in numerical solution of ODE

tion y . The curves show the typical behavior of non-stiff equations.

For all numerical methods, there will be inevitably errors (both local error in each time step and global error at the end of calculation) in the calculations. Modern computer codes attempt to adjust the step size to control the size of some of these errors. The reference [18] mentioned three kinds of error measure:

- *local truncation error or local discretization error;*
- *local error;*
- *global error.*

The LLNL solver has an error calculation routine and it keeps the error within the tolerance limits prescribed by the user. It varies the time step automatically in order to maintain the required accuracy. I have tried different values of tolerances, tolerance values are varied from 10^{-2} to 10^{-8} . Theoretically, the smaller the tolerance value, the more accurate the solution was. When the tolerance was too small, for example when the tolerance value is 10^{-8} , the solver stopped the program because the tolerance limit was unacceptable. Finally, a tolerance of value 10^{-4} was selected.

The variation in time step does not influence the result too much, but it really affects the shape of the curves as shown in Figure (4.3). The LSODE solver automatically subdivides the time step into small steps according to the requirement of the tolerance.

Figure 4.2: Different initial values of f_s for single grain (time step = 0.4s). The initial value started from 10^{-20} to 10^{-12} (from right to left).

Figure 4.5: Different time step sizes of f_s for single grain. The time steps are 0.2s, 0.3s, 0.4s, 0.5s, 0.6s, 0.8s, 1.0s (from right to left).

The different starting initial values make some differences in the results.

Chapter 5

Results

In this chapter, the theory of equiaxed dendritic solidification is tested by comparing it with Rappaz's test example. Furthermore, the eutectic plateaus are also shown in our testing problems. We have tried to couple the solidification with a finite element analysis by using the residual method and trying different iteration times. Different boundary conditions have also been tested and all the results are presented below.

5.1 Rappaz's One-D casting problem

Rappaz has created a one dimensional casting problem [9]. The mesh has ten equi-lengthed two-node elements. The material is AL-7%Si. At one boundary, Rappaz described the boundary condition as zero flux. At the other end, he gave a chill condition. Rappaz's coupling strategy is shown by the following flow chart. From the flow chart we can see that, in fact, Rappaz didn't use iterations between the calculation of solidification and the calculation of heat field in FEM. Rappaz has created a one-D problem, the mesh is shown in fig. 5.2. His result is shown in figure 5.3. Rappaz has tested his numerical solution with measurements and they agreed, as shown in figure 5.4.

Figure 5.1: Flow chart of Rappaz's coupling method. Copied from Rappaz' paper [9]

One-D, 10 element, 11 node mesh

Figure 5.2: One-D, 10 element mesh

5.2 Comparison of Our result with Rappaz's

We have created nearly the same one-dimensional casting problem as Rappaz's did. We tried the problem in Smalltalk with same coupling strategy. The result is shown as fig. 5.5 (in this chapter, all results of one-D 10 element mesh problems are shown at nodes 1, 2, 3, 4, 5, 6, 7, 8, 9, 10). From the figure we can see the result agrees with Rappaz's numerical solution. The further calculation presents the eutectic plateaus at the eutectic temperature, when the liquidus composition of the material has reached the eutectic composition. This result is in agreement with the theory (see fig. 5.6).

The temperature versus distance curves are also shown in fig. 5.7.

Except using Rappaz's coupling method, we have also used the residual method to couple solidification with FEM. With this method, we have tested

Figure 5.3: Numerical solution of Rappaz's testing problem showing cooling curve at nodes 1 to 10. Mesh is shown in fig. 5.2. Copied from Rappaz' paper [9]

Figure 5.4: Comparison of numerical solution with measurements. The same problem as fig. 5.3. Copied from Rappaz' paper [9]

Figure 5.5: Smalltalk solution for ONE-D casting problem, mesh is shown in fig. 5.2, time step = 0.2s.

Figure 5.6: Eutectic plateaus with same mesh as fig. 5.5.

Figure 5.7: Temperature versus Distance, mesh is same as fig. 5.6, time step = 0.2s.

different iterations and got the results as presented from figure.(5.8) to figure (5.12).

Some slight bouncing problems occur with iteration, but the general tendency is still good. If more iterations are applied, fewer bouncing problems occurs. We also observed the development of mushy zone between the liquidus area and the solid area. At beginning, the mushy zone was small near the cooling boundary, then it grew larger and moved towards the center. This result is interesting and will be used in the future research (see figure 5.13).

Figure 5.8: Solution of residual method with iterations = 2, mesh is shown in fig. 5.2, time step = 0.5s.

Figure 5.9: Solution of residual method with iterations = 3, mesh is shown in fig. 5.2, time step = 0.5s.

Figure 5.10: Solution of residual method with iterations = 4, mesh is shown in fig. 5.2, time step = 0.5s.

Figure 5.11: Solution of residual method with iterations = 10, mesh is shown in fig. 5.2, time step = 0.5s.

Figure 5.12: Solution of residual method with iterations = 30, mesh is shown in fig. 5.2, time step = 0.5s.

a) 5.0s

b) 10s

c) 20s

d) 30s

e) 40s

f) 50s

Figure 5.13: The development of mushy zone at time of 5s, 10s, 20s, 30s, 40s, 50s. The mesh is shown in fig. 5.2.

5.3 Other Boundary Condition Solutions

We created other boundary conditions for the test problems:

- Convection boundary condition:

The one-D problem has the mesh and elements as mentioned above. At the two ends, we prescribe one side as flux equals zero while the other side we give a surface element with convection boundary condition. The calculated result is shown in figure 5.14.

- Casting problem with mold and resistant material:

In this problem, we use DIE K1A steel as mold material. Between the mold element and the melting element, we set a resistance material. The resistance material has thermal properties, such as thermal conductivity, which is very small, nearly 100 times smaller than the AL-7%Si, and the volumetric heat capacity is zero. This kind of resistance material acts as a gas film between the melting and the mold. We prescribe the temperature in the mold as 20° centigrade, and the temperature at the initial condition for melting is 630° centigrade. Using our nonlinear solver, the result is shown in figure 5.15.

Figure 5.14: Convection boundary condition. The mesh is shown in fig. 5.2, time step = 0.5s, iterations = 10.

Figure 5.15: Casting problem with mold interface resistance material for a 10 element mesh, time step = 0.5s, iterations = 10.

5.4 Discussion

In coupling solidification to FEM, two things are important. One is the time step for FEM and the other is the sizes of the mesh.

- The influence of the time step for FEM:

Because the calculation of temperature field with latent heat released by the process of solidification of the melt is a nonlinear problem, the time step for FEM is important. On the one hand, too small a time step will cause bouncing and reheating problems (as shown in Fig. 5.16). On the other hand, too large a time step will not resolve the solidification phenomena (see figure 5.18). Besides, when the time step for FEM is too large, numerical diffusion becomes important [9].

- The influence of mesh size:

For Rappaz's coupling method, i.e., the method without iteration between the macroscopic calculation of ΔH and the microscopic calculation of the associated ΔT and Δf_s , the convergence with mesh size is excellent, except when the mesh size is too large [9]. When using the residual method with iterations between the macroscopic and the microscopic calculations, the selection of mesh size is important. Fig. 5.19 is the result of a 10 element mesh, fig. 5.20 and 5.21 show a 20 element and a 40 element meshes, and fig 5.22, fig. 5.23 are the results of the 20 and 40 element meshes separately. From theses results we can see that when the mesh size is too large, the bouncing problem occurs.

Figure 5.16: Time step = 0.1s, mesh is shown in fig. 5.2, iteration = 4

Figure 5.17: Time step = 2.0s, mesh is shown in fig. 5.2, iteration = 4

Figure 5.18: Time step = 4.0s, mesh is shown in fig. 5.2, iteration = 4

Figure 5.19: 10 elements mesh (shown in fig. 5.2), time step = 1.0s, iteration = 4

One-D, 20 element (equisized), 21 node mesh

Figure 5.20: 20 element mesh, one-D problem

One-D, 40 element (equisized), 41 node mesh

Figure 5.21: 40 element mesh, one-D problem

Figure 5.22: Time step = 1.0s, iteration = 4, mesh is shown in fig. 5.20. Results are shown at nodes 2, 4, 6, 8, 10, 12, 14, 16, 18, 20.

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MICROCOPY RESOLUTION TEST CHART
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Figure 5.23: Time step = 1.0s, iteration = 4, mesh is shown in fig. 5.21. Results are shown at nodes 4, 8, 12, 16, 20, 24, 28, 32, 36, 40

Chapter 6

Improved Rappaz's Model

Dr. Hughes has worked to improve Rappaz's model [23]. He has concentrated on the problem of the coupling of solidification to FEM, so that nonlinear solver can be used to solve this type of problem. A system of ODEs so is solved simultaneously to determine both the temperature field in the macroscopic calculation and the evolution of the fraction of solid in the microscopic calculation.

His model modifies the theory of Rappaz and is briefly described below.

6.1 Brief description of Hughes' Model

The enthalpy is given by:

$$H(T, f_s) = CT + L(1 - f_s) = \int_{T_{ref}}^T C_p dT + L(1 - f_s) \quad (6.1)$$

where T is temperature; f_s is the fraction solid; L is the latent heat coefficient; and C_p is volumetric heat capacity.

The heat equation governs the flow of heat by conduction (the only mechanism considered here) and is:

$$\dot{H} = \text{div}(\mathbf{k} \cdot \nabla T) + q \quad (6.2)$$

They present a version of the model suitable for incorporation into the heat equation, and make several approximations which will facilitate the numerical solution of the total model.

6.1.1 Nucleation

Dr. Hughes derived from M. Rappaz's model an expression to describe the rate of nucleation density.

$$\dot{n}(x, t) = -n'(\Delta T)Y^-$$

where the function Y^- is equal to Y if $Y \leq 0$, and to 0 if $Y > 0$.

6.1.2 Grain Growth

The room each grain has to grow in can be approximated by defining the radius R_{tot} as:

$$R_{tot}(x, t) = \left[\frac{3}{4\pi n(x, t)} \right]^{1/3}$$

R_{tot} is the average radius of the sphere of liquid surrounding each grain. It decreases with time until nucleation stops, and then becomes constant in time.

The time derivative $v = \dot{R}_g$ is assumed to be a function of ΔT only, i.e.,

$$\dot{R}_g = v(\Delta T)$$

where v is the velocity of dendrite tip growth. Then the R_g becomes:

$$R_g = R(\tau, t) = R(\tau, t, x) = \int_{\tau}^t v(\Delta T(x, s)) ds + R_c(\Delta T(x, \tau))$$

The initial radius R_c is a characteristic of the material, and depends on the value of ΔT at birth.

6.1.3 Volume of Solid and Time Derivative of f_s

Let f_i denote the volume fraction of solid of an individual grain, within the sphere of radius R_g , and let f_g denote the volume fraction of the inner sphere within the total outer sphere.

$$f_g = \frac{\frac{4\pi}{3} R_g^3}{\frac{4\pi}{3} R_{tot}^3} = \frac{4\pi}{3} R_g^3 n$$

Rappaz and Thevoz derived an expression for the internal solid fraction f_i of a grain, in terms of a model of diffusion from the grain envelope into the bigger sphere. The expression is, for a grain born in $[\tau, \tau + d\tau]$,

$$f_i^{(\tau)} = \min[1, \Omega(\Delta T(t))g(Z(\tau, t))] \quad (6.3)$$

where: $Z(\tau, t)$, $\Omega(\Delta T)$, k , $c^*(\Delta T)$, m , D , g have the same meaning as those in Rappaz's model.

The total volume solid, per unit volume, at time t , is:

$$f_s(x, t) = \frac{4\pi}{3} \int_0^t R(\tau, t)^3 \cdot \min[1, \Omega(\Delta T(t))g(Z)] \dot{n}(\tau) d\tau$$

Since they thought at this stage a fully developed dendritic structure formed, $\Omega g(Z)$ will be less than 1, so they have:

$$f_s = \frac{4\pi}{3} \int_0^t R(\tau, t)^3 \Omega(\Delta T(t))g(Z) \dot{n}(\tau) d\tau \quad (6.4)$$

The solute balance at this stage in a grain is expressed by:

$$\int_{V(g,t)} k c^*(y) dy + \left[\frac{4\pi}{3} R_g^3 - V(\tau, t) \right] c^* + 4\pi \int_{R_g}^{R_{tot}} c(r, t) r^2 dr = c_0 \left(\frac{4\pi}{3} R_{tot}^3 \right) \quad (6.5)$$

where $c(r, t)$ is the concentration in the spherical shell between R_g and R_{tot} , and where the notation $\int_V$ means the integral over the solid region. Differentiating this relation with respect to time and dividing by $(k - 1)C^*$ gives:

$$-\dot{V} + \left[\frac{4\pi}{3} R(\tau, t)^3 - V(\tau, t) \right] \dot{\Omega} + \frac{4\pi R(\tau, t)^2 D c_r(R(\tau, t), t)}{(1 - k)C^*} = 0$$

Follow Rappaz and Thevoz in approximating $c_r(R_g, t)$ by twice the average slope, $-\frac{c^* - c_0}{\delta/2}$, and taking $\delta = 2D/v$, they get:

$$-\dot{V} + \left[\frac{4\pi}{3} R(\tau, t)^3 - V(\tau, t) \right] \dot{\Omega} + 4\pi \Omega R(\tau, t)^2 v = 0 \quad (6.6)$$

f_s is expressed as follows:

$$f_s = \int_0^t V(\tau, t) \dot{n}(\tau) d\tau$$

By differentiating this, the rate of f_s is:

$$\dot{f}_s = \int_0^t \frac{\partial V(\tau, t)}{\partial t} \dot{n}(\tau) d\tau$$

Substituting the expression from (6-6):

$$\dot{f}_s = \dot{\Omega} \left[\frac{4}{3} \pi \int_0^t R(\tau, t)^3 \dot{n}(\tau) d\tau - f_s \right] + 4\pi \Omega \int_0^t R(\tau, t)^2 \dot{n}(\tau) d\tau v \quad (6.7)$$

They adopt some notation, for a non-negative integer j , they define:

$$P_j(t) = \int_0^t R(\tau, t)^j \dot{n}(\tau) d\tau$$

Then it is easily verified that:

$$\dot{P}_j(t) = R_c(t)^j \dot{n}(t) + jv(t) P_{j-1}(t)$$

Now $P_0(t) = n(t)$, and we can express (6-7) as:

$$\dot{f}_s = \dot{\Omega} \left[\frac{4\pi}{3} P_3 - f_s \right] + 4\pi \Omega v P_2 \quad (6.8)$$

6.1.4 Approximation of $g(Z)$ and Transition

1). Approximation of $g(Z)$

Recall that Rappaz and Thevoz's paper [6], [7], started from the solute balance, and introduced a correction function, $g(z)$,

$$g(z) = z + 1.5z + z^2 + 0.25z^4$$

Hughes made an approximation, they thought $R'_g - R_g$ to be a fixed proportion α of the diffusion layer thickness δ , and choose α to satisfy approximately the solute balance constraint. Using this assumption, they finally obtained:

$$f'_g = f_g(1 + \alpha Z)^3$$

Replacing $g(Z)$ by $(1 + \alpha Z)^3$ in (6-4) gives a simplified formula for f_s : let $w(t) = \alpha\delta = 2D\alpha/v(t)$. Then:

$$\begin{aligned} f_s &\approx \frac{4\pi}{3}\Omega \int_0^t R(\tau, t)^3 (1 + \alpha Z(\tau, t))^3 \dot{n}(\tau) d\tau \\ &= \frac{4\pi}{3}\Omega \int_0^t [R(\tau, t)^3 + w(t)]^3 \dot{n}(\tau) d\tau \end{aligned} \quad (6.9)$$

define:

$$Q(t) = \int_0^t [R(\tau, t)^3 + w(t)]^3 \dot{n}(\tau) d\tau$$

It is clear the approximation to f_s is equal to $\frac{4\pi}{3}\Omega(t)Q(t)$. Because $w(t)$ does not involve τ , one can write:

$$Q = P_3 + 3P_2w + 3P_1w^2 + nw^3$$

2). Transition from spherical to dendritic growth.

Compare the solute balance in spherical and dendritic stages, the value of concentration gradient for the former one is:

$$Dc_r = -(1 - k)c^*v = -(c^* - kc^*)v$$

and for the latter one is:

$$Dc_r = -(c^* - c_0)v$$

The transitional stage is characterized by the change in the gradient from the first to the second value. Represent it as a smooth transition by a "blending function", and assume that it is controlled by the comparison between $\Omega g(Z(\tau, t))$ and 1. Hughes represents the transition as:

$$Dc_r = -[c^* - (1 - \lambda)kc^* - \lambda c_0]v$$

where λ varies smoothly from 0 to 1. Considering f_s as $\frac{4\pi}{3}P_3$ in the spherical stage, and as $\frac{4\pi}{3}\Omega(t)Q(t)$ in the dendritic stage, the ratio $\rho(t) = P_3/(\Omega(t)Q(t))$ serves as a measure of the progress of transition. This ratio approaches 0 as t approaches 0, and when its value is 1, the transition is thought to be complete. With this idea, one can use $\rho(t)$ to determine λ . As an example, we might use the blending function:

$$\lambda(\rho) = \begin{cases} 0 & \text{for } \rho < 0 \\ (1/2)(1 - \cos(\rho * \pi)) & \text{for } 0 \leq \rho \leq 1 \\ 1 & \text{for } \rho > 1 \end{cases}$$

6.1.5 Impingement and After

As the dendrite tips approach the boundary of R_{tot} , the concentration gradient in the liquid outside the R_j becomes shallower, this is because the

diffusion layer begins to hit the outer shell. As a result, diffusion slows until the concentration is effectively uniform through out the radius R_{tot} . The impingement starts. Again from the solute balance, Hughes got the expression:

$$\dot{f}_s = \dot{\Omega} \left[\frac{4\pi}{3} P_3 - f_s \right] + 4\pi \Omega \varphi(t) v P_2 \quad (6.10)$$

where $\varphi(t)$ is a blending function that makes the transition from $R_g + \delta = R_{tot}$ to $R_g \rightarrow R_{tot}$ smooth. After the concentration gradient is reduced to 0, the liquid is uniform throughout the sphere of radius R_{tot} . The solute balance equation then reduces to:

$$\int_{V(\tau,t)} k c^*(y) dy + \left[\frac{4\pi}{3} R_{tot}^3 - V(\tau,t) \right] c^* = \frac{4\pi}{3} c_0$$

Differentiating with respect to time, multiplying by $\dot{n}$ and integrating with respect to τ , we get:

$$-\dot{f}_s + \dot{\Omega}(1 - f_s) = 0 \quad (6.11)$$

$$\frac{\dot{f}_s}{(1 - f_s)} = \dot{\Omega}$$

integrate it:

$$f_s = 1 - K/e^{\Omega} \quad (6.12)$$

6.1.6 Coupling to the Heat Equation

Coupling the solidification to the heat equation and noting those transitions, Hughes and Goldak finally reached a system of ODEs as:

For $\varphi(t) > 0$ and $T \geq T_{eut}$:

$$\begin{aligned} [C + L\Omega'(\Delta T) \left[\frac{4\pi}{3} P_3 - f_s \right]^+] \dot{T} &= \text{div}(k \nabla T) + q \\ &\quad + 4\pi L[(1 - \lambda) + \lambda \Omega] \varphi(t) v(\Delta T) P_2 \\ \dot{P}_3 + R_c(\Delta T)^3 n'(\Delta T) \dot{T}^- &= 3v(\Delta T) P_2(t) \\ \dot{P}_2 + R_c(\Delta T)^2 n'(\Delta T) \dot{T}^- &= 2v(\Delta T) P_1(t) \\ \dot{P}_1 + R_c(\Delta T) n'(\Delta T) \dot{T}^- &= v(\Delta T) n(\Delta T) \end{aligned} \quad (6.13)$$

For $\varphi(t) = 0$ and $T \geq T_{eut}$:

$$\begin{aligned} [C + L\Omega'(\Delta T)(1 - f_s)]\dot{T} &= \text{div}(\mathbf{K}\nabla\mathbf{T}) + \mathbf{q} \\ f_s &= 1 - K/e^\Omega \\ \Omega &= \Omega(\Delta T) \end{aligned} \quad (6.14)$$

After eutectic trasformation starts, for $T < T_{eut}$:

$$C\dot{T} = \text{div}(\mathbf{K}\nabla\mathbf{T}) + \mathbf{q} + LC_{fs}(T_E - T)^2 \quad (6.15)$$

where C_{fs} is a constant from the relation:

$$C_{fs} = \frac{f_s}{\Delta t} \frac{1}{\Delta T^2}$$

The detail description and theory can be seen in Dr. Hughes' report [23].

6.2 Algorithm in the program

We ignored R_c , i.e., $R_c = 0$.

$$V_{velocity} = a_2(\Delta T)^2$$

Where a_2 is a material constant. For $\dot{T} < 0$

$$n' = 6n_{max} \frac{\Delta T}{\Delta T_{nmax}^2} \left(1.0 - \frac{\Delta T}{\Delta T_{nmax}} \right)$$

$$\dot{n} = -n'\dot{T}$$

$$n = n_{max} \left(\frac{\Delta T}{\Delta T_{nmax}} \right)^2 \left(3 - 2 \frac{\Delta T}{\Delta T_{nmax}} \right)$$

For $\dot{T} > 0$

$$\dot{n} = 0$$

$$n = n_{max}$$

Where n is the grain density. ΔT_{nmax} is the maximum undercooling at which all nuclei are active, n_{max} is the maximum grain density.

$$R_{tot} = \left[\frac{3}{4\pi n} \right]^{1/3}$$

$$\dot{P}_1 = V_{velocity} n$$

$$\dot{P}_2 = 2V_{velocity} P_1$$

$$\dot{P}_3 = 3V_{velocity} P_2$$

Use Forward Euler Method to solve this set of ODEs simultaneously to get the value of P_1 , P_2 , P_3 at time $t + \Delta t$.

$$C^* = C_0 - \frac{\Delta T}{m}$$

where m is the the slope of liquidus.

$$\Omega = \frac{C^* - C_0}{(1 - k)C^*}$$

Where k is the partition coefficient.

$$\Omega' = -\frac{C_0}{(1 - k)mC^{*2}}$$

$$\omega = \frac{2D\alpha}{V_{velocity}}$$

$$Q = P_3 + 3P_2\omega + 3P_1\omega^2 + \omega^3$$

$$\rho = \frac{p_3}{Q\Omega}$$

$$\begin{cases} \lambda = 0 & \text{for } \rho < 0 \\ \lambda = (1/2)(1 - \cos(\rho\pi)) & \text{for } 0 \leq \rho \leq 1 \\ \lambda = 1 & \text{for } \rho > 1 \end{cases}$$

Under the condition that $\lambda < 1$ we have:

$$f_s = \frac{4}{3}\pi P_3$$

$$H_{eat} = 0.0$$

$$H_{eatsource} = 4\pi L((1 - \lambda) + \lambda\Omega)V_{velocity}P_2$$

For $\lambda \geq 1$, we need to calculate the value of ϕ

$$\delta = \omega/\alpha$$

$$R_g = P_1/n$$

$$\gamma = R_g + \delta - R_{tot}$$

$$\begin{cases} \phi = 1 & \text{for } \gamma < 0 \\ \phi = \frac{(1-2\gamma/\delta)}{(1-\gamma/\delta)^4} & \text{for } 0 \leq \gamma \leq \delta/2 \\ \phi = 0 & \text{for } \gamma > \delta/2 \end{cases}$$

For $\phi > 0$

$$f_s = \frac{4\pi}{3}Q\Omega$$

$$K = (1 - f_s)\Omega$$

$$H_{eat} = L\Omega'[\frac{4\pi}{3}P_3 - f_s]^+$$

$$H_{eatsource} = 4\pi L((1 - \lambda) + \lambda\Omega)\phi V_{velocity}P_2$$

For $\phi \leq 0$

$$f_s = 1 - K/e^\Omega$$

$$H_{eat} = L\Omega'(1 - f_s)$$

$$H_{eatsource} = 0$$

When the temperature drops to the eutectic temperature or the composition of the solute at the outer surface of R_g reaches the eutectic composition,

the solidification goes into the eutectic mode. It is just like phase 4 or impingement discussed in chapter 3. We have:

$$\dot{f}_s = C_{fs}(T_{eut} - T)^2$$

in which:

$$C_{fs} = \frac{f_s}{\Delta t} \left(\frac{1}{\Delta T_{eut}} \right)^2$$

with the restriction that:

$$\dot{f}_s \leq \frac{1 - f_s}{\Delta T}$$

The heat equation is:

$$C_p \dot{T} = \dot{H} + L \dot{f}_s$$

6.3 Test results

We have implemented FORTRAN code to check that the growth of f_s correspond to the temperature decrease. Fig. 6.1 to fig. 6.3 show different growth time (in seconds) with different cooling rates.

Coupling this model of solidification with FEM by using residual method, we tested the same one-D problem as mentioned in chapter 5. The results are shown in Fig. 6.4.

Figure 6.1: Fraction solid f_s with cooling rate = $-2\text{ }^{\circ}\text{C/sec.}$ (single grain)

Figure 6.2: Fraction solid f_s with cooling rate = $-10\text{ }^{\circ}\text{C/sec}$. (single grain)

Figure 6.3: Fraction solid f_s with cooling rate = $-50\text{ }^{\circ}\text{C/sec.}$ (single grain)

Figure 6.4: Time step= 0.2s, mesh is shown in fig. 5.2, iteration= 4

Chapter 7

Conclusion and Future Work

In this chapter, we will discuss the research work we have done, and compare the results from both Rappaz's model and the improved Rappaz's model. The effects of the different time steps and mesh sizes, as well as the number of iterations used in coupling solidification to FEM heat equation is also considered. Finally we will discuss the opportunities for future work and research in this field.

7.1 Discussion of present work

7.1.1 Rappaz' Model

Rappaz's model is good in reflecting the physical phenomena of equiaxed dendritic solidification process. It is also easy to establish the mathematical model. Rappaz did not show clearly those stages such as nucleation, spherical growth and impingement. He focused on the most important part of dendritic growth.

On the other hand, we have given a complete description of the Four phases of the equiaxed dendritic solidification, from nucleation; spherical growth; dendritic growth; and impingement.

As well, we have established the mathematical model corresponding to the four stages of the grain growth.

The major advantages of Rappaz's model are listed below:

1. Using Rappaz's Coupling Method.

Rappaz's coupling method [9] lacks iterations between macroscopic calculation of the increment of enthalpy, ΔH , and the microscopic calculation of the associated increment of fraction of solid, Δf_s , and increment of temperature, ΔT . So this method really does not cause the bouncing and reheating problems as other methods do. Rappaz said the result from the method agrees with the real measurement.

2. The Eutectic plateau.

When the temperature drops down to the eutectic temperature, or as an alternative, the concentration at the outer face of grain, C^* , reaches the value of eutectic concentration, then phase 4, impingement starts. The physical phenomenon at this stage of solidification is that there appears a flat curve or a constant line of temperature, eutectic plateau. Based on Rappaz's model, our calculation in phase 4, reflects this phenomenon very well in both single grain growth and the coupling solidification to FEM heat equation.

One of the disadvantages of Rappaz's model is when coupling the solidification with FEM heat equation by using iterations between macroscopic and microscopic calculations, the bouncing problem occurs, though we tried different mesh sizes and different length of time steps.

The other point is that the model is complicated and so the computational time is long time in calculation. This will be a prominent concern when

using this model to calculate large castings. It will be even worse if we try more iterations between macroscopic and microscopic calculations.

7.1.2 Improved Rappaz' Model

Hughes' model has kept the advantage of reflecting the physical process of equiaxed dendritic solidification. Furthermore, because of the use of blending functions, the transfer from one stage to another goes smoothly. Besides Hughes' model is simpler. So one of its advantage is that it saves computing time. The whole solidification process is reflected only in one short expression, and the four-phases transfer is done by two blending functions.

Hughes' model is designed for coupling solidification to FEM heat equation. All the phenomena, heat flow from the liquidus to the mold or ambient surroundings, nucleation, grain growth, and latent heat release happened simultaneously. Therefore, it is supposed to represent the real process of solidification more truly than the old model.

Unfortunately, we encountered bouncing problem again when we tried to introduce the iterations between macroscopic and microscopic calculations as can be seen in those figures in the previous chapter. This is because the mesh is too coarse.

There is another problem for Hughes' model. We calculate the heat equation and solidification simultaneously, compared with Rappaz's coupling method that lacks iterations between the macroscopic and microscopic calculations. However, to describe the solidification process, we have to use small time step. Now a problem arises, on the one hand, we need to use a large time

step to avoid bouncing and to speed the calculation in solving the heat equation. On the other hand, we have to use small time steps to accurately resolve the phenomena of the solidification process. This is a contradiction. The computing time by using this model to solve a real casting problem may be too much.

7.2 Future Work

The calculation of equiaxed dendritic solidification is important in real casting problem. At present, we can follow its evolution by the mathematical prescription, but as mentioned above, it costs too much CPU time to calculate a real casting. As well in the coupling, there are the problems of bouncing and reheating, which occur when introducing the iterations between the calculations of macroscopic heat field and microscopic development of solidification. One of the areas of future work for us to pursue is to try to solve the coupling problem. In the topic of solidification, some new methods are worth developing, though they might not describe the solidification evolution in detail as Rappaz's model did. They could give the characteristics of general development of solidification, and more importantly, they could provide the necessary tools for the calculation of the heat field. Consequently, they could solve the real casting problems with great efficiency.

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