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Study of solidification, shrinkage and natural convection in casting processes

Chen, Yin-Heng, Ph.D.
The Ohio State University, 1990
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PUBLICATIONS


FIELDS OF STUDY

Major field: Engineering Mechanics
Studies in Finite Element Analysis, Solidification Analysis, Creep Analysis, Post-buckling Analysis and Solid Mechanics
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACKNOWLEDGMENTS</td>
<td>ii</td>
</tr>
<tr>
<td>VITA</td>
<td>iii</td>
</tr>
<tr>
<td>LIST OF FIGURES</td>
<td>vi</td>
</tr>
<tr>
<td>LIST OF TABLES</td>
<td>xii</td>
</tr>
<tr>
<td>NOMENCLATURE</td>
<td>xiii</td>
</tr>
<tr>
<td><strong>CHAPTERS</strong></td>
<td></td>
</tr>
<tr>
<td>I INTRODUCTION</td>
<td>1</td>
</tr>
<tr>
<td>1.1 Review of Literature</td>
<td>2</td>
</tr>
<tr>
<td>1.2 Research Objectives and Outline</td>
<td>4</td>
</tr>
<tr>
<td>II FINITE ELEMENT MODELING OF SOLIDIFICATION</td>
<td>8</td>
</tr>
<tr>
<td>2.1 Finite Element Modeling of Heat Transfer</td>
<td>8</td>
</tr>
<tr>
<td>2.2 Time Discretization</td>
<td>12</td>
</tr>
<tr>
<td>2.3 Treatment of the Latent Heat of Solidification</td>
<td>15</td>
</tr>
<tr>
<td>2.3.1 Enthalpy Method</td>
<td>15</td>
</tr>
<tr>
<td>2.3.2 Fictitious Heat-Flow Method</td>
<td>19</td>
</tr>
<tr>
<td>2.3.3 Temperature Recovery Method</td>
<td>20</td>
</tr>
<tr>
<td>2.3.4 Front Tracking Method</td>
<td>22</td>
</tr>
<tr>
<td>III THEORETICAL BASIS OF SHRINKAGE PREDICTION</td>
<td>24</td>
</tr>
<tr>
<td>3.1 Review of Literature in Shrinkage Prediction</td>
<td>24</td>
</tr>
<tr>
<td>3.2 Prediction of Macro-shrinkage</td>
<td>29</td>
</tr>
<tr>
<td>3.3 Porosity Prediction</td>
<td>32</td>
</tr>
<tr>
<td>IV TWO-DIMENSIONAL ANALYSES OF SOLIDIFICATION</td>
<td>35</td>
</tr>
<tr>
<td>4.1 Case One - Axisymmetric Sand Casting of Steel</td>
<td>36</td>
</tr>
<tr>
<td>4.2 Case Two - Sand Casting of Steel Piston Crown</td>
<td>43</td>
</tr>
<tr>
<td>4.3 Case Three - Low Pressure Die Casting of</td>
<td>51</td>
</tr>
<tr>
<td>Aluminum Alloy Wheel</td>
<td></td>
</tr>
<tr>
<td>Section</td>
<td>Title</td>
</tr>
<tr>
<td>---------</td>
<td>----------------------------------------------------------------------</td>
</tr>
<tr>
<td>4.4</td>
<td>Case Four - Evaluation of Heat Transfer Coefficient for a Steel Mold Aluminum Casting</td>
</tr>
<tr>
<td>V</td>
<td>FINITE ELEMENT MODELING OF MOMENTUM, HEAT AND SPECIES TRANSPORT</td>
</tr>
<tr>
<td>5.1</td>
<td>Literature Survey</td>
</tr>
<tr>
<td>5.2</td>
<td>Solidification with Natural Convection by Front Tracking Method</td>
</tr>
<tr>
<td>5.3</td>
<td>Solidification with Natural Convection by Temperature Recovery Method</td>
</tr>
<tr>
<td>5.4</td>
<td>The Heat, Momentum and Species Transport in a Binary Solidification System</td>
</tr>
<tr>
<td>VI</td>
<td>THREE DIMENSIONAL APPLICATIONS OF SOLIDIFICATION PROBLEMS</td>
</tr>
<tr>
<td>6.1</td>
<td>Case Five - Temperature in a Cubic with a Prescribed Temperature Boundary Condition</td>
</tr>
<tr>
<td>6.2</td>
<td>Case Six - Temperature in a Cubic with a Convective Boundary Condition</td>
</tr>
<tr>
<td>6.3</td>
<td>Case Seven - Temperature in a Semi-infinite Plane with Phase Change</td>
</tr>
<tr>
<td>6.4</td>
<td>Case Eight - Solidification of a Corner Region</td>
</tr>
<tr>
<td>6.5</td>
<td>Case Nine - Comparison of Different Methods</td>
</tr>
<tr>
<td>VII</td>
<td>CONCLUSIONS</td>
</tr>
<tr>
<td>7.1</td>
<td>Concluding Remarks</td>
</tr>
<tr>
<td>7.2</td>
<td>Future Research Recommendations</td>
</tr>
<tr>
<td>REFERENCES</td>
<td></td>
</tr>
<tr>
<td>APPENDICES</td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>EIGHT-NODE THREE-DIMENSIONAL ELEMENT</td>
</tr>
<tr>
<td>B</td>
<td>CALCULATION OF TOTAL SHRINKAGE CAVITY</td>
</tr>
<tr>
<td>C</td>
<td>RELATIONSHIP BETWEEN G/R^{1/2} PRESSURE DROP</td>
</tr>
<tr>
<td>D</td>
<td>CONTINUUM MODEL FOR MOMENTUM, HEAT AND SPECIES TRANSPORT IN A BINARY ALLOY SYSTEM</td>
</tr>
</tbody>
</table>
### LIST OF FIGURES

<table>
<thead>
<tr>
<th>FIGURE</th>
<th>PAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>2. 1</td>
<td>Schematic diagram for solid, liquid and mold.</td>
</tr>
<tr>
<td>2. 2</td>
<td>Phase transition zone in a quadrilateral 4-node element after [5].</td>
</tr>
<tr>
<td>3. 1</td>
<td>Comparison of isotherms for alloys with narrow (a) and wide (b) freezing range.</td>
</tr>
<tr>
<td>3. 2</td>
<td>Dendritic structure and critical solid fraction ratio.</td>
</tr>
<tr>
<td>3. 3</td>
<td>Sketch illustrating an isolated nonsolid zone and void formation.</td>
</tr>
<tr>
<td>4. 1</td>
<td>Geometry for Case One, an axisymmetric steel casting [24] (All dimensions are in millimeters, not to scale).</td>
</tr>
<tr>
<td>4. 2</td>
<td>Temperature distributions in casting and sand mold for Case One at time = 30 minutes; liquidus temperature = 1525°C; solidus temperature = 1494°C.</td>
</tr>
<tr>
<td>4. 3</td>
<td>Temperature distributions in casting and sand mold for Case One at time = 90 minutes; liquidus temperature = 1525°C; solidus temperature = 1494°C.</td>
</tr>
<tr>
<td>4. 4</td>
<td>Comparison of Shrinkage Prediction for Case One between calculated F.E.M. simulation and experiment in [24].</td>
</tr>
<tr>
<td>4. 5</td>
<td>Geometry and locations of temperature measurements for Case Two, given in reference [25] (All dimensions are in millimeters).</td>
</tr>
<tr>
<td>4. 6(a)</td>
<td>Temperature distribution in the casting for Case Two at time = 6 minutes; liquidus temperature =1522°C; solidus temperature = 1492°C.</td>
</tr>
<tr>
<td>4. 6(b)</td>
<td>Temperature distribution in the casting for Case Two at time = 30 minutes; liquidus temperature =1522°C; solidus temperature = 1492°C.</td>
</tr>
<tr>
<td>4. 6(c)</td>
<td>Temperature distribution in the casting for Case Two</td>
</tr>
</tbody>
</table>
at time = 60 minutes; liquidus temperature = 1522°C; solidus temperature = 1492°C. ................................................. 49

4. 6(d) Temperature distribution in the sand mold for Case Two at time = 60 minutes; liquidus temperature = 1522°C; solidus temperature = 1492°C. ................................................. 50

4. 7 Comparison of temperature history at four measuring points (see Fig. 4.5 for locations). ................................................. 52

4. 8 Comparison of shrinkage for Case Two between computed F.E.M. prediction and experiment [25], (shrinkage ratio = 4.08%). ................................................................. 53

4. 9 Cross section of low pressure aluminum wheel die casting (Case Three) (Position 1-6 represent the locations for temperature measurement in [62]). ................................................. 54

4. 10 Initial temperature distribution and thermal resistance conditions (After reference [62]). ................................................. 57

4. 11(a) Temperature distribution in the casting for Case Three at time = 30 seconds with temperature interval = 10°C; liquidus temperature = 610°C; and solidus temperature = 572°C. ................................................................. 58

4. 11(b) Temperature distribution in the casting for Case Three at time = 45 seconds with temperature interval = 10°C; liquidus temperature = 610°C; and solidus temperature = 572°C. ................................................................. 59

4. 11(c) Temperature distribution in the casting for Case Three at time = 300 seconds with temperature interval = 10°C; liquidus temperature = 610°C; and solidus temperature = 572°C. ................................................................. 60

4. 12 Temperature distribution in the steel mold for Case Three at time = 300 seconds with temperature interval = 25°C; liquidus temperature = 610°C; and solidus temperature = 572°C. ................................................................. 61

4. 13 Calculated $G / \sqrt{R}$ for Case Two (Cross-hatched represents the zone where $G / \sqrt{R} < 1$). The dimension of $G / \sqrt{R}$ is in ($\text{deg min})^{1/2} / \text{cm.}$ ............... 64
<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.14</td>
<td>Configuration of the experiment and locations of measurement.</td>
<td>67</td>
</tr>
<tr>
<td>4.15</td>
<td>Calculated heat transfer coefficients by minimizing Equation (4-2) and assumed heat transfer coefficients by Equation (4-3). (Unit is cal/m² sec °C).</td>
<td>69</td>
</tr>
<tr>
<td>4.16</td>
<td>Comparison between predicted and experimental temperatures. Predicted values were calculated by minimizing Equation (4-2).</td>
<td>70</td>
</tr>
<tr>
<td>4.17</td>
<td>Comparison between predicted and experimental temperatures. Predicted values were calculated by minimizing Equation (4-3).</td>
<td>72</td>
</tr>
<tr>
<td>5.1</td>
<td>Schematic of solid-liquid interface in a solidifying system.</td>
<td>78</td>
</tr>
<tr>
<td>5.2</td>
<td>Schematic diagram of a two-element domain.</td>
<td>83</td>
</tr>
<tr>
<td>5.3</td>
<td>Dimensions and boundary conditions for solidification with natural convection effect.</td>
<td>89</td>
</tr>
<tr>
<td>5.4(a)</td>
<td>Vector plot of the velocity field for Ra₁=10⁵ at time = 171 seconds.</td>
<td>90</td>
</tr>
<tr>
<td>5.4(b)</td>
<td>Vector plot of the velocity field for Ra₁=10⁵ at time = 512 seconds.</td>
<td>91</td>
</tr>
<tr>
<td>5.5(a)</td>
<td>Temperature distribution for Ra₁=10⁵ at time = 171 seconds with the temperature interval=5°C.</td>
<td>92</td>
</tr>
<tr>
<td>5.5(b)</td>
<td>Temperature distribution for Ra₁=10⁵ at time = 512 seconds with the temperature interval=5°C.</td>
<td>93</td>
</tr>
<tr>
<td>5.6</td>
<td>Velocity vector field for Ra₁=10⁴ at time = 512 seconds.</td>
<td>94</td>
</tr>
<tr>
<td>5.7</td>
<td>Temperature distribution for Ra₁=10⁴ at time = 512 seconds with the temperature interval=5°C.</td>
<td>95</td>
</tr>
<tr>
<td>5.8</td>
<td>Solid/liquid interfaces for different Rayleigh numbers at time = 512 seconds.</td>
<td>97</td>
</tr>
<tr>
<td>5.9</td>
<td>Temperature distributions along x axis at time = 171 seconds without the natural convection effect.</td>
<td>98</td>
</tr>
<tr>
<td>5.10</td>
<td>Geometry and temperature distributions along the half height at 2 minutes after solidification starts</td>
<td>VIII</td>
</tr>
</tbody>
</table>
with $T_l=34^\circ\text{C}$, $T_h=34^\circ\text{C}$, $T_c=12.5^\circ\text{C}$.

5.11 Velocity vector and temperature distribution at 0.238 minutes after solidification starts with $T_l=34^\circ\text{C}$, $T_h=34^\circ\text{C}$, $T_c=12.5^\circ\text{C}$.

5.12 Velocity vector and temperature distribution at 2.33 minutes after solidification starts with $T_l=34^\circ\text{C}$, $T_h=34^\circ\text{C}$, $T_c=12.5^\circ\text{C}$.

5.13 Quasi uniform (A) and graded (B) mesh layout.

5.14(a) Velocity field by temperature recovery method for $Ra=10^5$ at time = 512 seconds.

5.14(b) Temperature distribution by temperature recovery method for $Ra=10^5$ at time = 512 seconds; temperature interval = 5°C.

5.15 Vertical velocity by employing mesh A, mesh B, and front tracking method.

5.16 Velocity vector and temperature distribution by temperature recovery method for $Ra=10^5$ at time = 171 seconds (Four cold wall with temperature 510°C).

5.17 Velocity vector and temperature distribution by temperature recovery method for $Ra=10^5$ at time = 445 seconds (Four cold wall with temperature 510°C).

5.18 Temperature distributions without natural convection at time = 445 seconds (Four cold wall with temperature 510°C).

5.19 Dimensions and thermal boundary conditions for the rectangular ingot casting of Al-4.4%Cu alloy.

5.20 Temperature distribution (rectangular ingot casting of Al-4.4%Cu alloy at 53 seconds; temperature interval=10°C).

5.21 Velocity vector (rectangular ingot casting of Al-4.4% Cu alloy at 53 seconds).

5.22 Composition distribution (rectangular ingot casting
of Al-4.4%Cu alloy at 53 seconds; temperature
interval=0.01). ................................................................. 127

5. 23 Dimensions for the square ingot casting of
Al-4.4%Cu alloy. .............................................................. 128

5. 24 Temperature distributions (solidification of Al-4.4%Cu
alloy at 16.95 seconds; temperature interval = 10°C; (a)
for heat conduction only. (b) for heat conduction and
convection, and (c) for conduction, convection and
species transport). ............................................................. 130

5. 25 Velocity vectors (solidification of Al-4.4%Cu alloy at
16.95 seconds; (a) for heat conduction and convection,
and (b) for conduction, convection and species
transport). ......................................................................... 131

5. 26 Shrinkage distributions ((a) for heat conduction only.
(b) for heat conduction and convection, and (c) for
conduction, convection and species transport). ................. 132

6. 1 Comparison between analytical and F.E. results
calculated with Δt=0.001 sec. for a prescribed
temperature boundary condition. ................................. 138

6. 2 Comparison between analytical and F.E. results
calculated with Δt=0.001 sec. for a heat flux
boundary condition. ......................................................... 140

6. 3 Configuration and boundary conditions of Case Seven. 141

6. 4 Analytical and F. E. temperature history at x=2.54 cm
of a semi-infinite phase change problem (Case Seven). 141

6. 5 Analytical and F. E. temperature along x axis at time 1
second of a semi-infinite phase change problem
(Case Seven). ............................................................... 144

6. 6 Mesh and boundary conditions for Case Eight. .......... 146

6. 7 Front position along 45° bisectrix for Case Eight. ...... 148

6. 8 Temperature history at location x=y=0.5 m for
Case Eight. ................................................................. 149

6. 9 Finite element model for Case Nine ...................... 151
6. 10  Temperature distribution along x axis of Case Nine. . . . . 153
A. 1  The position of nodal point for 8-node linear element. . . 169
C. 1  Model of porosity formation. ................................. 174
# LIST OF TABLES

<table>
<thead>
<tr>
<th>TABLE</th>
<th>PAGE</th>
</tr>
</thead>
<tbody>
<tr>
<td>4. 1</td>
<td>Simulation conditions for an axisymmetric steel casting. 38</td>
</tr>
<tr>
<td>4. 2</td>
<td>Thermal properties of steel (Case One). 39</td>
</tr>
<tr>
<td>4. 3</td>
<td>Thermal properties of Chromite sand (Case One). 39</td>
</tr>
<tr>
<td>4. 4</td>
<td>Simulation conditions for Case Two. 45</td>
</tr>
<tr>
<td>4. 5</td>
<td>Thermal properties of Silica sand and exothermic powder for Case Two. 46</td>
</tr>
<tr>
<td>4. 6</td>
<td>Thermal properties of steel and aluminum alloy for Case Three. 55</td>
</tr>
<tr>
<td>4. 7</td>
<td>Experimental and calculated solidification time in sec. 62</td>
</tr>
<tr>
<td>5. 1</td>
<td>Thermal properties of aluminum. 88</td>
</tr>
<tr>
<td>5. 2</td>
<td>Dimensionless parameters for aluminum. 88</td>
</tr>
<tr>
<td>5. 3</td>
<td>Thermal properties of Al-4.4%Cu. 124</td>
</tr>
<tr>
<td>5. 4</td>
<td>Comparison of solidification and C. P. U. times for five different cases of solidification. 134</td>
</tr>
<tr>
<td>6. 1</td>
<td>Material properties, boundary conditions and initial conditions for Case Nine. 151</td>
</tr>
<tr>
<td>6. 2</td>
<td>Computer runs in Case Nine. 152</td>
</tr>
<tr>
<td>A. 1</td>
<td>The location and node number for each surface of at 8-node element. 169</td>
</tr>
</tbody>
</table>
NOMENCLATURE

Alphabet Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>surface area</td>
</tr>
<tr>
<td>$\bar{B}$</td>
<td>spatial gradient matrix of shape functions</td>
</tr>
<tr>
<td>$\bar{B}_{1,2}$</td>
<td>spatial gradient matrix in x and y directions</td>
</tr>
<tr>
<td>c</td>
<td>heat capacity</td>
</tr>
<tr>
<td>$\bar{C}$</td>
<td>heat capacity matrix</td>
</tr>
<tr>
<td>$C_L$</td>
<td>characteristic length</td>
</tr>
<tr>
<td>$d_1$</td>
<td>primary dendrite arm spacing</td>
</tr>
<tr>
<td>$d_2$</td>
<td>secondary dendrite arm spacing</td>
</tr>
<tr>
<td>D</td>
<td>diffusion coefficient</td>
</tr>
<tr>
<td>E</td>
<td>internal energy</td>
</tr>
<tr>
<td>f</td>
<td>composition</td>
</tr>
<tr>
<td>$f_L$</td>
<td>volume fraction of liquid</td>
</tr>
<tr>
<td>$f_{\alpha}$</td>
<td>composition of constituent $\alpha$ in liquid phase</td>
</tr>
<tr>
<td>$f_{\alpha, e}$</td>
<td>eutectic composition of constituent $\alpha$ in liquid phase</td>
</tr>
<tr>
<td>$f_s $</td>
<td>volume fraction of solid</td>
</tr>
<tr>
<td>$f_v $</td>
<td>volume fraction of void</td>
</tr>
<tr>
<td>h</td>
<td>boundary heat transfer coefficient</td>
</tr>
<tr>
<td>g</td>
<td>gravity</td>
</tr>
<tr>
<td>G</td>
<td>thermal gradient</td>
</tr>
<tr>
<td>k</td>
<td>heat conductivity</td>
</tr>
<tr>
<td>K</td>
<td>permeability</td>
</tr>
</tbody>
</table>
L : latent heat of solidification
L_r : feeding distance
M : mass
N : shape function matrix
P : dynamic pressure
Pr : Prandtl number
R : local cooling rate
Ra_T : Rayleigh number
Ra_C : Solutal Rayleigh number
Ste : Stefan number
t : time
T : temperature
T_e : eutectic temperature
u, v : components of velocity
U* : surface interpolation matrix
w : weighted factor in Gauss quadrature formula

Greek Alphabet Symbols
\(\alpha\) : thermal diffusivity
\(\beta\) : volume shrinkage ratio due to solidification
\(\beta_c\) : solutal expansion coefficient
\(\beta_T\) : thermal expansion coefficient
\(\beta\) : volume shrinkage ratio due to solidification
\(\lambda\) : penalty constant
\[ \mu \quad : \quad \text{kinematic viscosity} \]
\[ v \quad : \quad \text{dynamic viscosity} \]
\[ \theta \quad : \quad \text{non-dimensionalized temperature} \]
\[ \rho \quad : \quad \text{mass density} \]
\[ \Gamma \quad : \quad \text{boundary} \]
\[ \Omega \quad : \quad \text{domain} \]
\[ \xi, \eta, \zeta \quad : \quad \text{coordinate for three-dimensional element} \]
CHAPTER I
INTRODUCTION

Knowledge of temperature history, position of solid and liquid boundaries, temperature gradients, and liquid velocities is very important for casting engineers in predicting formation of voids, porosity, macro-segregation, and micro-structures. This type of predictive capability is very useful in reducing casting defects without carrying out a costly and tedious trial-and-error procedure. The main objective of this study is to analyze the solidification process for pure metals or binary alloys with the effects of natural convection, interdendritic flow and species transport.

Few analytical solutions are available for solidification problems due to mathematical difficulties. One of the major complexities is the release of the latent heat of solidification during phase change which occurs at the fixed-melting temperature for pure metals or a range of temperatures (liquidus and solidus) for metal alloys. The release of latent heat and microstructure growth may be coupled with the diffusion at the liquid-solid interface. Both the nucleation mechanism and the diffusion near the interface will influence the temperature distribution. Therefore, temperature is not the only variable in the solidification problem. In the present study, the effect of nucleation has not been considered but the momentum and mass transport in the liquid and mushy zone has been considered.

Finite element techniques are employed for the analysis of two-dimensional and axisymmetric solidification processes to predict temperature
history and shrinkage and porosity distributions. A single step implicit time stepping method is employed for numerical time integration. The effects of natural convection and species transport have been studied also. The incompressibility condition is enforced by employing the penalty method. In handling the release of latent heat, both the temperature recovery method and the front tracking method are studied and compared. The results show that the temperature recovery method is suitable for solving solidification problems for pure metals as well as alloys with or without natural convection. The two-dimensional program has been further extended to three-dimensional geometries. Some preliminary results which compare well with other known solutions are discussed.

1.1 Review of Literature

Mathematical theories for phase change problems have been studied for a long time. However, analytical solutions are limited to some special geometries and boundary conditions. One major problem dealing with phase change is the treatment of the release of latent heat. To handle the release of latent heat, many researchers have developed different techniques such as the enthalpy method [1-7], the fictitious heat-flow method [8], the temperature recovery method [9-11] and the front tracking method [12-13]. Some comparisons of the results obtained from these techniques have been made in references [14-17]. Although the temperature recovery method may not be the most accurate method, it is still a good candidate because it is reasonably accurate and easy to adopt for a wide range of applications.
For the prediction of macro-shrinkage, Jeyarajan et al. [18] and Henzel et al. [19] used equi-solidification methods and Bishop et al. [20] developed a temperature gradient technique. Some empirical rules have also been used in predicting wave front using a modulus-based technique [21,22]. Moosbrugger and Berry [23] correlated the feeding distance to the centerline shrinkage. Imafuku et al. [24,25] developed a mathematical model for shrinkage prediction.

Microporosity prediction has been performed by Piwonka et al. [26] and Kubo et al. [27]. They proposed a mathematical modeling of pressure drop to predict porosity. Niyama et al.[28,29] used a parameter in terms of thermal gradient and cooling rate to predict the formation of voids. According to their work, quantitative prediction of porosity is very difficult to obtain unless detailed information about interdendritic flow and associated pressure drop at mushy zones is available.

Interface heat transfer coefficients are introduced to simulate the complex heat transfer mechanism across the casting/mold interface. A survey of heat transfer coefficients has been made by Papai and Mobley [30]. The heat transfer coefficients have been represented as functions of location and time due to gap formation at the mold/casting interface [31-35]. Some authors [36,37] have determined the heat transfer coefficients by minimizing the square mean error between calculated and measured temperatures from thermocouples. A similar technique is employed in this study to determine heat transfer coefficients.

Finite difference techniques and the enthalpy method [1,38-40] have been used to solve solidification problems for pure metals including the effects of natural convection in the liquid pool. Gartling [41] and Yoo and
Rubinsky [13] performed a similar work using a finite element technique. Desai et al. [42] simulated the forced and natural convection during the filling stage of a casting. Experimentally determined temperature field and phase front of the solidification for gallium [43] and tin [44] whose melting temperatures are low, have been compared to the computed results in this study. The presence of a mushy zone makes the calculation of fluid flow more complex. Many researchers [45-49] simulated the interdendritic flow using Darcy's rule. The permeability was calculated as a function of fraction of solid in mushy zone. To solve the heat, momentum and species transport of a binary alloy solidifying system, Bennon and Incropera [50] introduced a continuum model. They also used the finite difference method and upwinding technique [45,51] to solve the solidification problem in a rectangular cavity. Experimental results for an aqueous solution of ammonium chloride were compared with numerical solutions obtained by the finite difference method [52,53].

1.2 Research Objectives and Outline
The objective of this study is to investigate computational methods for a solidifying system with a special consideration of phase change. Computational efficiency and accuracy are also studied. Mathematical models dealing with the heat, momentum and mass transport are constructed for the simulation of a solidifying process. In the mushy zone, Darcy's law is applied to simulate the interdendritic flow. Then, the computed temperature distribution is used in predicting the shrinkage and the formation of pores.
In chapter 2, two- and three-dimensional finite element formulations are developed. An implicit method of time integration is employed in the present study to ensure numerical stability. An investigation of four different methods of treating the latent heat effect is made. The temperature recovery method is employed for the second part of the study because it is construed to be computationally more adaptable than other methods. A technique to handle the thermal resistance and gap formation at the coincident nodes in the mold/casting interface is also discussed.

The theoretical basis of shrinkage and porosity prediction is described in chapter 3. The shrinkage prediction is performed under the assumption that gravity is the main driving force and that a critical solid fraction ratio exists in the mushy zone. The calculation procedure includes the summation of the change in solid fraction ratio in the nonsolid zone for each time step and distributes the shrinkage to proper elements. The void formation is predicted when the pressure drop at the mushy zone is greater than some critical value obtained from experiments. The numerical procedure involves the calculation of the thermal gradients and local cooling rate.

Two-dimensional applications of the developed program are made in Chapter 4 by ignoring natural convection effects in the liquid pool. The temperature distributions of steel sand casting (Cases one and two), low pressure die casting (Case three) and permanent mold casting (Case four) are calculated and compared to experimental results available from the literature. Shrinkage and porosity are also predicted and compared with experimental results in Cases one and two. Generally speaking, the agreement between the experimental and computed results were reasonably good. Since the interface conditions will vary, different heat transfer coefficients are adopted at several
locations for a low pressure die casting problem (Case three). In Case four, the heat transfer coefficient is evaluated by minimizing the errors between the calculated and measured temperatures.

A general solidification model, including the effect of natural convection, interdendritic flow, and species transport is discussed in chapter 5. A literature survey is presented in section 5.1. The derivation of a continuum model for momentum, heat and species transport in a binary solidification system is discussed in section 5.2. The solidification of pure metal in a rectangular enclosure including the natural convection effect is studied by using both the front tracking method and the temperature recovery method. The numerical results suggest that a refined mesh must be employed when the temperature recovery method is used. The computed temperature distribution during the solidification of gallium is compared with experimental measurements. It shows good agreement. The investigation is extended to solve a binary solidification system with interdendritic flow and species transport. The interdendritic flow is modelled as Darcy's flow while the species transport is considered in the liquid and mushy zone. Effects of natural convection, species transport and heat transfer coefficients on the temperature, shrinkage and total solidification time are studied at the end of Chapter 5.

The last topic in this study concerns the extension of the developed program and the temperature recovery method to three-dimensional applications in Chapter 6. The momentum equations are not considered. Four cases are studied to verify the developed program. Firstly, the heat conduction in a cube with prescribed temperature and heat flux boundary conditions was calculated. The computed temperature distributions were
compared with the analytical solutions from the literature. Good agreements are found in both cases. The solidifications of a semi-infinite bar and the corner freezing problem are also studied with three-dimensional meshes. Comparisons between the computed and analytic solutions show that good agreement can be obtained if proper time increments are selected. The temperature history of a semi-infinite solidification problem by enthalpy, front tracking and temperature recovery methods are also compared.

The conclusions of this research and several future recommendations are presented in chapter 7.

One of the main objectives of this study is to extend the temperature recovery method for the simulation of a solidifying system including natural convection. The developed program is applied in studying shrinkage and porosity formation during the solidification. Effects of mushy zone size and species transport are also studied. It is hoped that the finite element simulation of a general solidification problem would become more effective through this kind of study.
CHAPTER II
FINITE ELEMENT MODELING OF SOLIDIFICATION

Some theoretical background of finite element modeling of solidification processes are discussed in this chapter. The derivations of two- and three-dimensional finite element formulations of the heat conduction problem are given in Section 2.1. Section 2.2 describes several types of time discretization techniques. Numerical techniques for treating the release of latent heat during solidification are discussed in Section 2.3.

2.1 Finite Element Modeling of Heat Transfer

In this section, a general procedure for applying the finite element model to unsteady heat conduction is described. The model discussed in this section neglects the effects of convection in the molten metal. Natural convection and species transport are considered in Chapter V.

The partial differential equations of heat conduction can be expressed as

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + Q$$  \hspace{1cm} (2-1)

with boundary conditions,

$$T = T_w \hspace{1cm} \text{on} \hspace{0.5cm} \partial \Omega_1 , \hspace{1cm} (2-2)$$

$$-k \frac{\partial T}{\partial n} = q_n + q_c + q_r \hspace{0.5cm} \text{on} \hspace{0.5cm} \partial \Omega_2 , \hspace{1cm} (2-3)$$
\[-k \frac{\partial T}{\partial n} = h \left( T_{\text{metal}} - T_{\text{mold}} \right) \quad \text{on} \quad \partial \Omega_3, \quad (2-4)\]

\[k_s \frac{\partial T_s}{\partial n} - k_l \frac{\partial T_l}{\partial n} = \rho L \frac{\partial X}{\partial t} \quad \text{on} \quad \Gamma \quad (2-5)\]

where \( \vec{n} \) is the unit outward normal vector, \( T \) temperature, \( \rho c \) the heat capacity, \( k \) the thermal conductivity, and \( Q \) the rate of internal heat generation. The boundary \( \partial \Omega_1 \) is the temperature prescribed boundary, while \( \partial \Omega_2 \) is the heat flux prescribed boundary where \( q_n \), \( q_c \) and \( q_r \) are the imposed heat flux and the rates of heat flux due to convection and radiation, respectively, which can be expressed as \( q_c = h_c (T - T_\infty) \) and \( q_r = h_r (T - T_\infty) \) where \( T_\infty \) is the ambient temperature. Here, \( h_c \) and \( h_r \) denote the effective heat transfer coefficients due to convection and radiation, respectively. The boundary \( \partial \Omega_3 \) is the convective boundary condition at the mold and casting interface in which \( h \) is the interfacial heat transfer coefficient. \( T_{\text{metal}} \) is the temperature at the surface of casting and \( T_{\text{mold}} \) is the temperature at the mold surface. In Equation (2-5), \( \Gamma \) represents the phase interface and subscripts \( s \) and \( l \) are used for the thermal properties of the solid phase and the liquid phase, respectively. \( \rho L \partial X \) is the heat release per unit area when the surface of the phase interface moves a distance \( \partial X \), \( \vec{n} \) is the outward unit normal to the phase front. A schematic representation of this problem is shown in Figure 2.1.

Following the standard finite element formulation in references [54,55], the unknown temperature \( T \) can be approximated over the domain \( \Omega \) by a combination of interpolation functions:

\[T(\vec{x}, t) = \sum_{i=1}^{n} T_i(t) N_i(\vec{x}) \quad (2-6)\]
Figure 2.1. Schematic diagram for solid, liquid and mold
where \( n \) is number of nodes per element, \( N_i(x) \) are the shape functions and \( T_j(t) \) are the nodal temperatures. By applying the weak formulation and the Green-Gauss theorem to Equation (2-1), one can get a system of ordinary differential equations of the following form,

$$
\ddot{\bar{C}}(T) \dot{T} + (\bar{K}_k(T) + \bar{K}_n(t')) \bar{T} = \bar{Q}_q + \bar{Q}_2 + \bar{Q}_3.
$$

(2-7)

Here, \( \bar{C} \) and \( \bar{K}_k \) denote the \((n \times n)\) heat capacity and conductivity matrices, respectively, and \( \bar{K}_n \) denotes the matrix containing the effects of the convective boundary condition. \( \bar{Q}_q \) represents the internal heat generation vector, \( \bar{Q}_2 \) and \( \bar{Q}_3 \) are the vectors from the heat flux on the surfaces of \( \partial \Omega_2 \) and \( \partial \Omega_3 \), respectively. The superposed dot refers to differentiation with respect to time. The matrix elements and vectors are of the form,

$$
\bar{C} = \int_\Omega \rho c \bar{N}^T \bar{N} \, dV ,
$$

$$
\bar{K}_k = \int_\Omega k \nabla \bar{N}^T \cdot \nabla \bar{N} \, dV ,
$$

$$
\bar{K}_n = \int_{\partial \Omega} h \bar{N}^T \bar{N} \, dS ,
$$

(2-8)

and

$$
\bar{Q}_q = \int_\Omega \bar{N}^T Q \, dV ,
$$

$$
\bar{Q}_2 = \int_{\partial \Omega_2} \bar{N}^T (q_n + q_c + q_r) \, ds ,
$$

$$
\bar{Q}_3 = \int_{\partial \Omega_3} \bar{N}^T h T_{\text{mold}} \, ds .
$$

(2-9)

The shape functions, Jacobian of a 3D eight-node element and procedures for numerical integration are given in Appendix A.
In handling the convective boundary condition along the casting/mold interface, a thin interface element [5] or coincident node technique [56] can be used along interface. The coincident node technique is employed in this study for the flexibility in the mesh generation.

### 2.2 Time Discretization

Two classes of time discretization methods will be discussed: one-step method (two-time-level) and two-step method (three-time-level). The general form of the one-step method for time integration of Equation (2-7) is,

$$ T^{n+1} = K^{n+1} T^{n+1} + Q^{n+1} + T_n + p - T_n + p $$

The two level scheme interpolates these matrices and vectors by those at the temporal points $n$ and $n+1$ with a parameter $\omega$:

$$
\begin{align*}
\bar{C}^{n+1} &= \omega \bar{C}^{n+1} + (1-\omega) \bar{C}^n \\
\bar{K}^{n+1} &= \omega \bar{K}^{n+1} + (1-\omega) \bar{K}^n \\
\bar{Q}^{n+1} &= \omega \bar{Q}^{n+1} + (1-\omega) \bar{Q}^n \\
\bar{T}^{n+1} &= \omega \bar{T}^{n+1} + (1-\omega) \bar{T}^n \\
T &= (T^{n+1} - T^n) / \Delta t
\end{align*}
$$

where $\Delta t$ indicates the time increment and $0 \leq \omega \leq 1$. If $\omega = 0$, the method is said to be explicit. If the capacity matrix is diagonal, the recurrence formula (2-10) can be advanced without solving the matrix. If $\omega \neq 0$, the method is said to be implicit. It is well known that the Crank-Nicolson method ($\omega = 0.5$) and the Euler backward finite difference method ($\omega = 1$) are special cases of
the one-step method. Unconditional stability can be achieved when $\omega \geq 0.5$ [54]. The implicit formula is expressed by:

$$
[\bar{C} - \omega \Delta t \bar{K}]^{n+\omega} \bar{T}^{n+1} = [\bar{C} + (1 - \omega)\Delta t \bar{K}]^{n+\omega} \bar{T}^{n} + \Delta t \bar{Q}^{n+\omega}.
$$

(2-12)

A general form of the three level method can be written as,

$$
\bar{C}^*(\bar{T}^{n+1} - \bar{T}^{n-1})/\Delta t + \bar{K}^*[(\frac{1}{2} + a)\bar{T}^{n+1} + (\frac{1}{2} - 2a)\bar{T}^{n} + a\bar{T}^{n-1}] = \bar{Q}^*
$$

(2-13)

where $0 \leq a \leq 1$ and the superscript * indicates the quantities evaluated at time

$$
t^* = t_{n+1/2}.
$$

(2-14)

The Dupont II scheme [57,58], with $a=1/4$, was found to have no oscillations and high accuracy in solving heat conduction problems. The general form is,

$$
(\bar{C}^* + \frac{3}{4}\Delta t \bar{K}^*) \bar{T}^{n+1} = \bar{C}^* \bar{T}^{n-1} - \frac{1}{4}\Delta t \bar{K}^* \bar{T}^{n-1} + \Delta t \bar{Q}^*.
$$

(2-15)

The matrices are evaluated at $t^* = \frac{3}{2}t_n - \frac{1}{2}t_{n-1}$. The second scheme is Lees algorithm [59] which has the following recurrence form:

$$
(\bar{C}^{n} + \frac{2\Delta t}{3}\bar{K}^{n})\bar{T}^{n+1} = -\frac{2\Delta t}{3}\bar{K}^{n}\bar{T}^{n} + (\bar{C}^{n} - \frac{2\Delta t}{3}\bar{K}^{n})\bar{T}^{n-1} + \frac{2}{3}\Delta t \bar{Q}^{n}.
$$

(2-16)

Some comparisons between these discretization schemes have been presented by Dalhuijsen and Segal [14] and Thomas et al. [15]. It is well known that the finite difference method is good for problems with simple geometries, saving computing time as well as computer storage. For problems with irregular geometries, the Euler, Crank-Nicolson and Dupont II schemes give better results than the Lees Algorithm. According to Dalhuijsen's results,
the Dupont II scheme is superior to Lees scheme in both accuracy and stability. The lumped heat capacity matrix is shown to achieve slightly better results and solution efficiency than the consistent capacity matrix. From the above discussion, one can find that either Euler backward or Crank-Nicolson method with a lumped heat capacity matrix will be a good choice to solve the transient heat-conduction problem. The implicit method with \( \omega = 1 \) is used in solving the solidification with natural convection because of its unconditional stability and accuracy.

The material properties \( c, \rho, \) and \( k \) in equations (2-8) and (2-9) may be functions of temperature and pressure. The dependence of coefficients \( c, \rho, \) and \( k \) on temperature makes equation (2-7) nonlinear. Equation (2-7) can be expressed as,

\[
\bar{L}'(T) = \bar{C}(T) \ddot{T} + \bar{K}(T)\dot{T} - \bar{Q}_q - \bar{Q}_2 - \bar{Q}_3 = 0. \tag{2-17}
\]

The well known Newton-Raphson iteration scheme is obtained by taking linear terms in the Taylor series expansion of equation (2-17) about a trial solution \( T_m^n \),

\[
T_0^n = T^n \\
T_{m+1}^n = T_m^n + \left( \frac{d}{dT} L'(T_m^n) \right)^{-1} L'(T_m^n), \quad m = 0, 1, 2 \ldots \tag{2-18}
\]

where \( m \) denotes the number of iterations. The Jacobian matrix has to be evaluated at every iteration which is very expensive to operate. In solving the momentum equations of the present natural convection study, a modified Newton-Raphson iteration procedure is adopted by updating the Jacobian for each time step.
2.3 Treatment of the Latent Heat of Solidification

Four different ways of handling the release of latent heat are discussed in this section. According to Crank [16], discrete methods can be categorized in two groups; fixed-domain method and front tracking method in which a moving grid is employed across the solid/liquid requiring a mesh generation in each time step. A recent literature survey by Salcudean et al. [17], provides some comparisons of these methods. According to the findings of Salcudean et al. [17] the enthalpy method (a fixed domain method) is reasonably accurate for the solidification of alloys. In addition, they found that the solution is relatively insensitive to the selection of time step and the size of mushy zone. Three methods based on the fixed-domain method and the front tracking method are briefly reviewed in the sequel.

2.3.1 Enthalpy Method

In this method, the transient part of the energy equation is expressed in terms of enthalpy instead of temperature. The enthalpy, including the release of latent heat, can be defined by,

\[ H = \int_{T_w}^{T_s} \rho c_s(T) dT + \int_{T_s}^{T} [\rho (dL/dT) + \rho c_f(T)] dT, \quad \text{for } T < T_s \]

\[ H = \int_{T_w}^{T_*} \rho c_s(T) dT + \int_{T_*}^{T_s} [\rho (dL/dT) + \rho c_f(T)] dT + \int_{T_s}^{T} \rho c_f(T) dT, \quad \text{for } T_s \leq T \leq T_1 \]  \hspace{1cm} (2-19)

\[ H = \int_{T_w}^{T} \rho c_s(T) dT + \rho L + \int_{T_*}^{T_s} \rho c_f(T) dT + \int_{T_s}^{T} \rho c_f(T) dT, \quad \text{for } T_1 \leq T \]

where \( c_s \) and \( c_f \) are the specific heat for solid and liquid phases, respectively. Here, \( c_f \) is the specific heat for \( T_s \leq T \leq T_1 \), \( L \) is the latent heat, and \( T_s \) and \( T_1 \)
are the solidus and liquidus temperatures, respectively. $T_{ref}$ is a reference temperature. With the above definitions of the enthalpy and with the assumption that the rate of internal heat generation is zero, the governing equation for the Stefan problem can be expressed as,

$$(\partial H / \partial t) - \nabla \cdot (k \nabla T) = 0,$$  \hspace{1cm} (2-20)

or by applying the chain rule,

$$(\partial H / \partial T) \left( \frac{\partial T}{\partial t} \right) - \nabla \cdot (k \nabla T) = 0. \hspace{1cm} (2-21)$$

The above equation represents the heat equation with a known temperature-dependent, "effective" heat capacity which accounts for the latent-heat effect. The effective heat capacity can be expressed as

$$c^* = \frac{dH}{dT},$$  \hspace{1cm} (2-22)

which results in, according to Equations (2-19),

$$c^* = \rho c_s,$$ \hspace{1cm} for \hspace{0.2cm} $T < T_s$,  

$$c^* = \rho c_f + \frac{L}{(T_f - T_s)}$$ \hspace{0.2cm} for \hspace{0.2cm} $T_s \leq T \leq T_f$,  \hspace{1cm} (2-23)

$$c^* = \rho c_l$$ \hspace{1cm} for \hspace{0.2cm} $T > T_f$,  

where the latent heat, $L$, is assumed to be homogeneous over the phase change zone. One major drawback of this method is that if the change of nodal temperature is larger than the given phase transition temperature regions, the latent heat effect will be ignored. This requires a fine mesh through the phase transition zone and/or some special techniques such as the use of discontinuous elements [4] and a locally adopted mesh [5,6], which may become computationally too demanding for pure materials or alloys with a
small mushy zone. Another drawback of the direct use of this effective heat capacity is that, in some cases, oscillation in the calculated temperatures may occur near the phase front unless a special numerical technique is devised [2,3].

Some averaging techniques are used to avoid the oscillation near the interface. Several methods of approximation have been developed to alleviate the numerical difficulties mentioned above. Among them, the methods of Del Giudice et al. [2], and Lemmon [3] have produced satisfactory results. Del Giudice et al. proposed to calculate the effective heat capacity by,

\[
c^* = \frac{[(\partial H / \partial x) (\partial T / \partial x) + (\partial H / \partial y) (\partial T / \partial y) + (\partial H / \partial z) (\partial T / \partial z)]}{[(\partial T / \partial x)^2 + (\partial T / \partial y)^2 + (\partial T / \partial z)^2]}
\] (2-24)

while Lemmon proposed

\[
c^* = \left[ \frac{[(\partial H / \partial x)^2 + (\partial H / \partial y)^2 + (\partial H / \partial z)^2]}{[(\partial T / \partial x)^2 + (\partial T / \partial y)^2 + (\partial T / \partial z)^2]} \right]^{1/2}
\] (2-25)

The presence of the spatial derivatives of the enthalpy and the temperature in the above expressions provides a smoothing effect so that oscillations near the phase front can be reduced in the finite element analysis.

Another technique treating the rapid change in the material property was introduced by Chen [4], which employs internally discontinuous elements along with a projection scheme to trace the phase transition zone.

In Figure 2.2, one can see a phase transition zone in a quadrilateral 4-node element. If the zone in an element, $\Omega^e_p$, bounded by the isotherms of $T_s$ and $T_l$, is assumed to be a phase transition zone, the energy balance in the element can be expressed as
Therefore, the local heat capacity matrix in the element that contains a liquid-solid interface is defined as

\[
(C)_i = \int_{\Omega} \rho \cN_j \cN_j d\Omega + \int_{\Omega} \rho L \frac{\dot{T}}{(T_1 - T_p)} d\Omega.
\] (2-27)

The second term in the above equation is the contribution of the latent heat release from the transition zone inside the element \(e\). With this modification, the enthalpy method can be applied to solidification modeling for either pure materials or metal alloys. Satisfactory results are reported by Kitamura [5] and Kitamura et al. [6] by coupling the technique with the multiple time stepping method and a locally adaptable mesh.

Figure 2.2. Phase transition zone in a quadrilateral 4-node element after [5].
2.3.2 Fictitious Heat Flow Method

The fictitious heat flow method [8] is applied iteratively along with the Euler-backward time integration scheme, Equation (2-12) with $\omega = 1$. One finds,

$$
(C^{n+1} - \Delta t K^{n+1})\bar{T}^{n+1} = C^n T^n + \Delta t \bar{Q}^{n+1}.
$$

(2-28)

Three vectors are used to control the progress of the phase front. The total latent heat flow available at a node $k$ is defined by,

$$
\bar{Q}_{\text{lat},k} = \int_{\Omega} \left( \frac{pL}{\Delta t} \right) N_k \, d\Omega.
$$

(2-29)

Here, $N_k$ is the temperature interpolation vector in an element and $\Delta t$ is the time interval. At the beginning of each time step, the fictitious heat flow vector, $\bar{Q}^{\circ}_{\text{lat},k}$ is initialized, i.e.,

$$
\bar{Q}^{\circ}_{\text{lat},k} = 0.
$$

(2-30)

Then, for each iteration $i$ within a time step, when the nodal temperature passes through the phase change temperature, the resulting heat-flow increment is calculated. Whenever the temperature passes through the melting temperature, the $i^{th}$ iteration of the incremental latent heat flow at a node $k$ is calculated by

$$
\Delta \bar{Q}_{\text{lat},k}^{i} = - \int_{\Omega} \left( \frac{\rho c^{n+1,i-1}}{\Delta t} \right) (T_{k}^{n+1,i} - T_m) N_k \, d\Omega
$$

(2-31)

where $T_m$ is the melting temperature and $n$ is the time step counter. The trial latent heat flow for the step is updated by,
Meanwhile, the nodal temperature in the process of solidification is fixed at the melting temperature of the material until solidification is completed:

\[
T_{k}^{n+1, i} = T_{m}.
\] (2-33)

The accumulation of latent-heat flow can be found from,

\[
\bar{Q}_{accu,k}^{i} = \bar{Q}_{accu,k}^{i-1} + \Delta Q_{int,k}^{i}.
\] (2-34)

over all iterations. This procedure is repeated until the accumulated latent-heat equates the total latent-heat flow available at the nodes. Then, the nodal temperatures are no longer fixed at \( T_{m} \) and the fictitious heat flow is no longer increased. When convergence is achieved, the next time step will start.

The procedure described here is applied to a pure material with a well defined melting temperature. A similar procedure can be applied to alloys with a certain freezing range. Details of the method can be found in Rolph and Bathe [8].

### 2.4.3 Temperature Recovery Method

The third method discussed is the temperature recovery method, classified as a fixed domain method, which requires no remeshing during the calculation. The basic procedure can be described in two steps. First, calculate the temperature distribution, \( T' \), without considering the latent heat effect. Then, the real temperature, \( T \), can be found by solving,

\[
\int_{T_{*}}^{T} \rho c dT + \int_{T_{*}}^{T} \rho L \left( \frac{\partial f_{s}}{\partial T} \right) dT = \int_{T_{*}}^{T} \rho c dT.
\] (2-35)
Here, \( T \) is the true temperature while \( T' \) is the temperature calculated without considering latent heat, and \( f_s \) is the fraction of solid.

Considering a volume element within the mushy zone, the energy release in that volume below the liquidus temperature at the time step, \( t + \Delta t \), can be determined by,

\[
Q = \int_{T_1}^{T_1 + \Delta t} \rho c V dT
\]  

(2-36)

where \( T_1 + \Delta t \) is the temperature at time step \( t + \Delta t \) without considering the latent heat and \( V \) is the volume of that element. In the numerical integration of Equation (2-36), the thermal properties at time step \( t \) are used in the present study.

Assuming that release of the latent heat of solidification during phase change is homogeneous, the energy balance in the solidifying region gives the modified actual temperature, \( T_{act}^{t+\Delta t} \) as follows,

\[
Q = \int_{T_1}^{T_1 + \Delta t} \left[ \rho c + \frac{L \rho}{T_1 - T_s} \right] V dT
\]  

(2-37)

or

\[
T_{act}^{t+\Delta t} = T_1 + \frac{(Q / V) (T_1 - T_s)}{[c(T_1 - T_s) + L] \rho}
\]  

(2-38)

where \( L \) is the latent heat of solidification.

This procedure continues until solidification is completed. The final solidification state can be determined by comparing the magnitude of energy release defined by \( Q \) in Equation (2-36) with the total release of heat during phase change, \( Q_T \) defined by,
When $Q$ is larger than $Q_T$ at a certain time $t'$, that particular volume element is considered to be solidified and the temperature is modified as,

$$T_{i}^{n'} = T_{i}^{n} + \frac{(Q + Q_{T}) / V}{(pc)_{s}}$$

where $(pc)_{s}$ is the heat capacity of the material at the solidus temperature.

For a fixed-melting temperature problem the present scheme can be easily extended by setting $T_{i} = T_{m} = T$ in Equations (2-38) and (2-40), where $T_{m}$ is the melting temperature of the material.

Hong et al. [9] solved solidification problems by the boundary element method and recovered the temperature by Equation (2-35). Tszeng et al. [10] and Im et al. [11] also adopted this method to get a reasonable temperature prediction of solidification processes. The time step is sensitive to the accuracy of prediction due to the nature of the temperature recovery method. From the results of comparison given in reference [17], it is construed that the temperature recovery method and fictitious heat method are less accurate than the enthalpy method.

### 2.3.4 Front Tracking Method

Unlike the three fixed domain methods introduced above, the front tracking method is a variable domain method. The front tracking method determines the new position of the interface by solving the energy balance equation (2-5) at the interface. Thus, the variables that need to be solved are nodal temperature as well as position of phase interface. The detailed finite
element formulation for Equation (2-5) can be found in references [12,13]. The basic procedure of this method is,

(1) solving the temperature distribution in the solid portion,
(2) solving the temperature distribution in the liquid portion,
and (3) solving the interfacial velocity from Equation (2-5).

From the results of Yoo and Rubinsky [12], accurate prediction of the position of phase front can be obtained with a coarse mesh. The solution is insensitive to mesh distribution and time step. Although there is no available comparisons between this method and other methods, the front tracking method has the capability to obtain quite accurate solutions since it satisfies the interfacial energy balance directly, accounting for the velocity of the liquid/solid phase interface. However, unlike the enthalpy method or the temperature recovery method, remeshing is required at almost every time step because the temperature distributions in the solid and liquid parts are solved separately at each time step. This disadvantage presents difficulties in adopting the method unless a sophisticated remeshing technique is available.
CHAPTER III
THEORETICAL BASIS FOR SHRINKAGE PREDICTION

In this chapter, techniques to predict shrinkage and porosity are discussed. A literature survey of shrinkage and porosity predictions is presented in section 3.1. Sections 3.2 and 3.3 present the theoretical background of Imafuku's technique for shrinkage prediction and the technique for porosity prediction using the parameter \( G/\sqrt{R} \), respectively.

3.1 Review of Literature in Shrinkage Prediction

Macro-shrinkage and porosity are the major defects in casting processes. The main reason for the macro-shrinkage is the failure in filling the mold during the casting process. Casting engineers have used many approaches such as risers on the top of casting to avoid the macro-shrinkage problem. On the other hand, porosity can result from either micro-shrinkage or gas diffusion. Micro-shrinkage can be caused by the limitation of the interdendritic feeding where the complexities of the dendritic structure make the filling process more difficult. Therefore, porosity often forms in the root of the dendritic structure. Another source of porosity is gas formation during cooling. Gas bubbles can develop from the melting processes, the reaction between the metal/mold interface, and turbulence during the filling stage [18-22,60].

24
Jeyarajan et al. [18] and Henzel et al. [19] used equi-solidification methods to predict shrinkage cavities. The positions of liquidus and solidus temperatures at various times were determined by numerical heat transfer analysis. Bishop et al. [20] developed a temperature gradient technique as a computer simulation method. The temperature gradient at the interface is a critical parameter for porosity prediction. Generally speaking, qualitative prediction of the shrinkage pattern can be made by utilizing information from heat transfer analysis. However, neither of these two methods predicted quantitatively the fraction of voids in the solidifying material.

Heine et al. [21] used a modulus-based technique to predict wave fronts by introducing some empirical equations. One example is Chvorinov's rule, \( \log t = C^* \log (V/A) \), where \( V/A \) is the section modulus, defined as the casting volume divided by its surface area where heat can be transferred out of the casting, \( t \) is the time to solidify, and \( C^* \) is a constant dependent on the material and the adopted units.

Davis and Magny [22] used a more complicated modulus-based technique to generate the shrinkage cavity profile for a given riser. Rollett and Lewis [60] analyzed the solidification of uranium alloy casting by using a commercially available finite element program ABAQUS. The castings were made in vacuum induction melting (VIM) casting system. They found that solidification front velocity is an important factor in predicting defects. The local solidification time, that is, the time required for a cell of material to cool from liquidus to solidus temperature, is a function of solidification front velocity and local temperature gradients. They mentioned several effects which the FEM simulation is incapable of predicting, namely:
(1) nucleation and growth behavior,
(2) temperature change resulting from segregation during dendritic growth,
(3) the transition from columnar to equiaxed microstructures.

Moosbrugger and Berry [23], concluded that, for narrow freezing range alloys, casting defect is primarily caused by the presence of centerline shrinkage, while for alloys with wide freezing ranges, "unsoundness" is primarily a dispersed interdendritic porosity, see Figure 3.1. They used the modified enthalpy equations to simulate some hypoeutectic characteristics of alloys. The feeding range was calculated and was found to be in good agreement with the results of Davis and Magny [22]. According to Davis et al., the feeding distance $L_f$ is,

$$L_f = \frac{B P_o r^2}{\mu m V_s}, \quad (3-1)$$

where $B$ is an empirical correction factor, $P_o$ is the pressure due to metallostatic head, $V_s$ is the solidification front velocity, $r$ is the radius of tube, $m$ is the solidification contraction, and $\mu$ is the liquid metal viscosity. By using the solid fraction along the center line, the capillary feeding distance can be determined.

Piwonka and Flemings [26] offered several approximate formulae for porosity prediction. They started with shrinkage in pure and nearly pure metals. They assumed a simple cylindrical groove in cellular solidification. Then, the pressure drop can be found as,

$$P_s - P_L = -\frac{8 \beta' U \mu L}{r^2} \quad (3-2)$$
Figure 3.1. Comparison of isotherms for alloys with narrow (a) and wide (b) freezing range.
where

\[ \beta' = \frac{\beta}{1 - \beta} \]

\( \beta \) = contraction due to solidification at solidifying temperature,

\( U \) = interface velocity (positive for solidification),

\( P_\ast \) = pressure at groove entrance,

\( P_L \) = pressure at root of groove,

\( \mu \) = viscosity of liquid,

and \( L \) = channel length.

For a more complicated model [26] for predicting shrinkage microporosity during dendritic solidification, the pressure drop can be determined as,

\[ P_\ast - P_L = \frac{32 \mu \beta' \lambda^2 L^2}{r^4} \left( \frac{t^2}{\pi R^2 n} \right) \]  

(3-3)

where

\( t \) = "tortuosity" factor that accounts for the fact that the liquid flow channels are not straight and smooth,

\( tL \) = effective channel length with \( t \geq 1 \),

\( n \) = number of flow channels per unit cross section of the cylinder,

\( R \) = radius of the cylinder,

and \( r \) = radius of liquid channel.

With this formula and the assumption that cavitation mediated voids form at zero absolute pressure, Piwonka and Flemings [26] predicted the size of the...
interdendritic porosity and obtained good agreement with the experimental results. Recently, Kubo et al. [27] also proposed a mathematical modeling of pressure drop in predicting porosity. According to the work mentioned above, a quantitative prediction of porosity is difficult to make unless detailed information on interdendritic flow and the associated pressure drop in the mushy zone is available.

3.2 Prediction of Macro-shrinkage

In the following, a numerical procedure for shrinkage cavity prediction will be presented, based on the work by Imafuku et al. [24,25] for steel castings. With this model, the macro-shrinkage and the fraction of voids can be predicted quantitatively. As a first step, expressions for the release of latent heat and solid fraction ratio as a function of temperature are introduced. An expression of solid fraction ratio as a function of temperature can be obtained from the Fe-C equilibrium diagram for steel castings. The solid fraction ratio, within the range of solidus and liquidus temperatures, can be assumed to change linearly with temperature. Four more assumptions are made as follows:

1. molten metal moves downwards with the force of gravity,
2. the speed of the molten metal flow is much higher than that of solidification,
3. the volume of shrinkage cavities is equal to the total volume contraction due to solidification,
(4) molten metal has full fluidity in a mushy zone, where the solid
fraction ratio is less than \( f_{cr} \), a critical solid fraction ratio."

The concept of \( f_{cr} \) could be obtained from the study of segregation [61].
From the dendritic structure as described in Figure 3.2, the solid fraction ratio
varies from 0 (at liquidus temperature) to 1 (at solidus temperature). As the solid fraction ratio increases, the dendritic structure links together making it more difficult for the liquid metal to flow. Referring to Figure 3.2, the "critical solid fraction ratio", \( f_{cr} \), can be introduced by observing the fact that the molten metal can move downwards by the gravitational force when solid fraction ratio is smaller than \( f_{cr} \) (region I). For region II whose solid fraction ratio is larger than \( f_{cr} \), the molten metal can not flow through the dendritic structure. Then, the shrinkage cavity volume \( \Delta V_v \), generated during a time step \( t \) at an isolated nonsolid region, can be determined from Equation (3-4), based on conservation of mass. The derivation of Equation (3-4) is given in Appendix B.

\[
\Delta V_v = \int_{V} \beta \rho_i \left\{ \left[ f_s|_{t=t} \left( 1 - v_s|_{t=t} \right) \right] - f_s|_{t=t-\Delta t} \left( 1 - v_s|_{t=t-\Delta t} \right) \right\} dV .
\]  

(3-4)

Here,

\( v_s|_{t=t} \) = the elemental shrinkage volume ratio per unit volume at
time step \( t \),

\( f_s|_{t=t} \) = solid volume fraction of infinitesimal region per unit volume
at time step \( t \),

\( \beta \) = the volume shrinkage ratio due to solidification,

\( \rho_i \) = material density for liquid state,
Figure 3.2. Dendritic structure and critical solid fraction ratio.
\( \rho_s \) = material density for solid state.

If there is more than one isolated nonsolid region, \( \Delta V_v \) needs to be calculated for each isolated nonsolid region.

The numerical procedure to determine shrinkage volume is as follows. Following the assumptions introduced above such that the molten metal moves downwards due to the gravitational force, the shrinkage cavity will be assumed to be distributed on top of each isolated nonsolid zone (depicted in Figure 3.3). For each element, the elemental shrinkage volume ratio, \( v^* \), is calculated at time step \( t \). Then, \( \Delta V_v \) is determined from Equation (3-4). The same amount of volume will be distributed to proper elements which are located on top of each of the isolated nonsolid zones. After that, the elemental shrinkage volume ratio will be determined and updated for each element in succeeding time step until the solidification is completed.

3.3 Porosity Prediction

Microporosity prediction is, in general, more difficult than shrinkage prediction. Imafuku et al. [24,25] found that (1) porosity tended to form at the regions which solidified last, and (2) as the thermal gradient at the end of solidification decreases, the porosity increases. This observation was correlated to a parameter \( G/\sqrt{R} \) (\( G \) is the temperature gradient and \( R \) is the cooling rate) at the end of solidification in casting and was introduced by Niyama et al. [28,29]. From these correlations it was concluded that lower thermal gradient induced the porosity formation.
Figure 3.3. Sketch illustrating an isolated nonsolid zone and void formation.
Niyama et al. found that the order of pressure drop at the root of dendrite was on the order of the parameter $G/\sqrt{R}$. Several assumptions were made to obtain this conclusion. The details of the derivation can be found in Appendix C. Furthermore, a critical value of $G/\sqrt{R}$ was determined to be one for low carbon steel from experiments. The criterion to determine the formation of porosity is that if $G/\sqrt{R} < 1$ void formation occurs and if $G/\sqrt{R} > 1$ void formation will not occur. This criterion has been used by several researchers and reasonable porosity prediction was obtained. This technique seems to be reliable in predicting porosity from casting processes for low carbon steel. However, more experimental work needs to be done to determine the critical values of $G/\sqrt{R}$ for other alloys.

In simulations, the thermal gradient and cooling rate at each time step was calculated using temperature distribution obtained from finite element program. At each nodal point in the mesh, the thermal gradient was computed at the certain time step when the nodal temperature moves through the liquidus temperature. The cooling rate was determined from the temperature difference between the present time step and the previous time step. For each node, the maximum thermal gradient in its neighboring nodes was used. Following these procedures, the porosity prediction was carried out. The numerical prediction of shrinkage and porosity for sand castings and pertinent comparisons with experimental data will be discussed in the next chapter.
CHAPTER IV
TWO-DIMENSIONAL ANALYSES OF SOLIDIFICATION
NEGLECTING NATURAL CONVECTION

A finite element program has been developed and applied for the simulation of two-dimensional and axisymmetric solidification processes. As described in Chapter 2, a contact thermal resistance was introduced for handling the interface heat transfer between molds and casting. The temperature recovery method was adopted for treating the release of latent heat. The techniques introduced by Imafuku et al. (Section 3.2) and Niyama et al. (Section 3.3) were used to predict the formation of macroshrinkage and porosity.

In this chapter, four examples are simulated to verify the accuracy and applicability of the developed finite element program and the shrinkage prediction scheme of solidification analyses. The first example is an axisymmetric steel casting. The second example is a piston crown steel casting with silica sand mold. The third case is an aluminum low pressure die casting. The fourth case is an axisymmetric aluminum casting with steel mold. In the fourth case, the heat transfer coefficients were evaluated by minimizing the errors between the calculated and measured temperatures. In Case Two, Three and Four, the calculated temperatures were compared with the measured temperature available in the literature.
4.1 Case One - Axisymmetric Sand Casting of Steel

The casting geometry is shown in Figure 4.1. The casting material was steel, with the following composition: 0.14%C, 0.43% Si, 0.78% Mn, 0.012%P, and 0.01%S (remainder is Fe, % represents wt%, here). The mold material was chromite sand. The calculation conditions are listed in Table 4.1. The thermal properties for steel and chromite sand used in simulations are given in Table 4.2 and 4.3, respectively. An effective heat transfer coefficient was assumed to be 0.1356 Kcal/m²·s °C throughout the casting/mold interface. The computed finite element solutions were not too sensitive to the size of time steps used in simulation (3 seconds and 12 seconds). However, since thermal gradient is very high at the interface, results from the coarse mesh (168 elements in casting and 324 elements in molds) were found to underestimate the temperature drop near the interface area when compared with the results from refined mesh (240 elements in casting and 620 elements in mold). It is suggested that more elements should be placed in large thermal gradient area.

The casting and mold temperature distributions employing the refined mesh after 30 minutes of solidification are shown in Figure 4.2, while those at 90 minutes are shown in Figure 4.3. Figure 4.2 shows temperature profiles at an earlier stage of solidification. Figure 4.3 shows the last location to solidify. It can be seen in Figure 4.3 that the heat extraction from the convex corner is much faster than that from the concave corner. In the mold, the high thermal gradient front will reach only about half the thickness of the mold. This means the temperature field at the outer half of mold does not change even though the solidification of the casting is almost finished. The corresponding result for the shrinkage prediction is shown in Figure 4.4 comparing with the experimental result obtained from the Imafuku's paper [24]. Good agreement
Figure 4.1. Geometry for Case One, an axisymmetric steel casting [24] (All dimensions are in millimeters, not to scale).
Table 4.1. Simulation conditions for an axisymmetric steel casting

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat transfer coefficient (sand-ambient)</td>
<td>0.0055</td>
</tr>
<tr>
<td>Ambient temperature</td>
<td>25.0</td>
</tr>
<tr>
<td>Latent heat (Kcal/Kg)</td>
<td>60.0</td>
</tr>
<tr>
<td>Critical solid fraction ratio</td>
<td>0.67</td>
</tr>
<tr>
<td>Initial temperatures</td>
<td></td>
</tr>
<tr>
<td>Metal temperature (°C)</td>
<td>1530</td>
</tr>
<tr>
<td>Sand temperature (°C)</td>
<td>25</td>
</tr>
<tr>
<td>Initial surface temperatures</td>
<td></td>
</tr>
<tr>
<td>Metal temperature (°C)</td>
<td>1524.5</td>
</tr>
<tr>
<td>Sand temperature (°C)</td>
<td>700</td>
</tr>
<tr>
<td>Liquidus &amp; solidus temperatures</td>
<td></td>
</tr>
<tr>
<td>Liquidus temperature (°C)</td>
<td>1525</td>
</tr>
<tr>
<td>Solidus temperature (°C)</td>
<td>1494</td>
</tr>
<tr>
<td>Solidification shrinkage ratio (%)</td>
<td>3.64</td>
</tr>
</tbody>
</table>
### Table 4.2. Thermal properties of steel (Case One)

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Thermal Conductivity (Kcal/m hr°C)</th>
<th>Heat Capacity (Kcal/Kg °C)</th>
<th>Density (Kg/m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt; 200</td>
<td>40.9</td>
<td>0.121</td>
<td></td>
</tr>
<tr>
<td>300</td>
<td>37.2</td>
<td>0.138</td>
<td></td>
</tr>
<tr>
<td>500</td>
<td>33.3</td>
<td>0.163</td>
<td></td>
</tr>
<tr>
<td>700</td>
<td>29.3</td>
<td>0.211</td>
<td>7500</td>
</tr>
<tr>
<td>900</td>
<td>25.5</td>
<td>0.180</td>
<td></td>
</tr>
<tr>
<td>1100</td>
<td>25.9</td>
<td>0.181</td>
<td></td>
</tr>
<tr>
<td>1200</td>
<td>26.7</td>
<td>0.192</td>
<td></td>
</tr>
<tr>
<td>&gt;1525</td>
<td>36.0</td>
<td>0.20</td>
<td>7000</td>
</tr>
</tbody>
</table>

### Table 4.3. Thermal properties of Chromite sand (Case One)

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Thermal Conductivity (Kcal/m hr°C)</th>
<th>Heat Capacity (Kcal/Kg °C)</th>
<th>Density (Kg/m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt; 200</td>
<td>0.709</td>
<td>0.170</td>
<td></td>
</tr>
<tr>
<td>300</td>
<td>0.663</td>
<td>0.180</td>
<td></td>
</tr>
<tr>
<td>500</td>
<td>0.674</td>
<td>0.188</td>
<td></td>
</tr>
<tr>
<td>700</td>
<td>0.724</td>
<td>0.195</td>
<td>2750</td>
</tr>
<tr>
<td>900</td>
<td>0.806</td>
<td>0.200</td>
<td></td>
</tr>
<tr>
<td>1100</td>
<td>0.937</td>
<td>0.205</td>
<td></td>
</tr>
<tr>
<td>1300</td>
<td>1.07</td>
<td>0.207</td>
<td></td>
</tr>
<tr>
<td>1400</td>
<td>1.13</td>
<td>0.209</td>
<td></td>
</tr>
</tbody>
</table>
Figure 4.2. Temperature distributions in casting and sand mold for Case One at time = 30 minutes; liquidus temperature = 1525 °C; solidus temperature = 1494 °C.
Figure 4.3. Temperature distributions in casting and sand mold for Case One at time = 90 minutes; liquidus temperature = 1525 °C; solidus temperature = 1494 °C.
Calculated Shrinkage Prediction (shrinkage ratio=3.64%)

Steel Casting (Case 1)
Time=117 Minutes

Critical solid fraction $f_{cr} = 0.67$

Void fraction ratio

$1.0 \rightarrow 0.95$
$0.95 \rightarrow 0.75$
$0.75 \rightarrow 0.50$
$0.50 \rightarrow 0.25$
$0.25 \rightarrow 0.01$
$0.01 \rightarrow 0.00$

Figure 4.4. Comparison of Shrinkage Prediction for Case One between calculated F.E.M. simulation and experiment in [24].
can be found in this figure when the calculated shrinkage is compared with the experimental observations.

4.2 Case Two - Sand Casting of Steel Piston Crown

The second example was a steel piston crown casting of a large-scale marine diesel engine with silica sand mold. The top of the riser was covered by an exothermic powder to reduce the rate of heat extraction from the riser. The cross section of piston crown and the positions of temperature measurement in reference [25] are shown in Figure 4.5.

Silica sand was used as the mold material and the casting metal was steel. The conditions of computation are given in Table 4.4. Table 4.5 shows the thermal properties of silica sand as well as those of the exothermic powder. The same thermal properties of steel as in Case One were used in this simulation. The mesh consisted of 236 and 391 quadrilateral elements in the casting and mold, respectively. Effective heat transfer coefficients were assumed to be 0.2712 Kcal/m² s °C in the outer casting/mold interface and 0.1356 Kcal/m² s °C in the inner casting/mold interface, respectively.

Figures 4.6(a), 4.6(b), and 4.6(c) illustrate the calculated temperature distributions in the casting at 6, 30, and 60 minutes after pouring, respectively. The calculated temperature distribution in the sand mold at 60 minutes after pouring is shown in Figure 4.6(d). It is seen in Figures 4.6(a) and 4.6(b) that the temperature distributions beneath the powder are different from those in other positions. This is due to the effect of the exothermic powder. In Figure 4.6(c), it was found that the location of highest temperature agrees closely with the location where porosities exist as observed in experiments [25]. This
Figure 4.5. Geometry and locations of temperature measurements for Case Two, given in reference [25] (All dimensions are in millimeters).
Table 4.4. Simulation conditions for Case Two

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat transfer coefficient (sand-ambient)</td>
<td>0.0055 Kcal/m² s °C</td>
</tr>
<tr>
<td>Ambient temperature</td>
<td>17.0 °C</td>
</tr>
<tr>
<td>Latent heat</td>
<td>60.0 Kcal/Kg</td>
</tr>
<tr>
<td>Critical solid fraction ratio</td>
<td>0.67</td>
</tr>
<tr>
<td>Initial temperatures</td>
<td></td>
</tr>
<tr>
<td>Metal</td>
<td>1530 °C</td>
</tr>
<tr>
<td>Sand</td>
<td>17 °C</td>
</tr>
<tr>
<td>Initial surface temperatures</td>
<td></td>
</tr>
<tr>
<td>Metal</td>
<td>1521.2 °C</td>
</tr>
<tr>
<td>Sand</td>
<td>700 °C</td>
</tr>
<tr>
<td>Liquidus &amp; solidus temperatures</td>
<td></td>
</tr>
<tr>
<td>Liquidus</td>
<td>1522 °C</td>
</tr>
<tr>
<td>Solidus</td>
<td>1492 °C</td>
</tr>
<tr>
<td>Solidification shrinkage ratio</td>
<td>4.08 %</td>
</tr>
</tbody>
</table>
Table 4.5. Thermal properties of Silica sand and exothermic powder for Case Two

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Thermal Conductivity (Kcal/m hr °C)</th>
<th>Heat Capacity (Kcal/Kg °C)</th>
<th>Density (Kg/m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Silica Sand</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>&lt; 200</td>
<td>0.663</td>
<td>0.213</td>
<td></td>
</tr>
<tr>
<td>300</td>
<td>0.581</td>
<td>0.224</td>
<td></td>
</tr>
<tr>
<td>500</td>
<td>0.562</td>
<td>0.233</td>
<td></td>
</tr>
<tr>
<td>700</td>
<td>0.592</td>
<td>0.240</td>
<td>1520</td>
</tr>
<tr>
<td>900</td>
<td>0.648</td>
<td>0.248</td>
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</tr>
<tr>
<td>1100</td>
<td>0.728</td>
<td>0.254</td>
<td></td>
</tr>
<tr>
<td>1300</td>
<td>0.796</td>
<td>0.258</td>
<td></td>
</tr>
<tr>
<td>1400</td>
<td>0.828</td>
<td>0.260</td>
<td></td>
</tr>
<tr>
<td>powder</td>
<td>0.036</td>
<td>0.20</td>
<td>200</td>
</tr>
</tbody>
</table>
Figure 4.6(a). Temperature distribution in the casting for Case Two at time = 6 minutes; liquidus temperature = 1522 °C; solidus temperature = 1492 °C.
continued Figure 4.6

Figure 4.6(b). Temperature distribution in the casting for Case Two at time = 30 minutes; liquidus temperature = 1522 °C; solidus temperature = 1492 °C.
continued Figure 4.6

Figure 4.6(c). Temperature distribution in the casting for Case Two at time = 60 minutes; liquidus temperature = 1522 °C; solidus temperature = 1492 °C.
Figure 4.6(d). Temperature distribution in the sand mold for Case Two at time = 60 minutes; liquidus temperature = 1522 °C; solidus temperature = 1492 °C.
verifies that the last place to solidify will be a possible location for porosity formation. Figure 4.6(d) also shows the high thermal gradient in the powder. The mold temperature in the inner core is higher than that in the outer part because the heat extraction from the outer mold surface was greater than that of the inner mold.

From these results, it was found that the developed program can be used to handle various boundary conditions such as chills, exothermic powders or paddings during solidification. Figure 4.7 compares the predicted temperature with experimental results at four locations, which shows good agreement except at P4. It is seen that the present F.E.M. program has the capability to predict temperatures accurately during solidification processes.

The shrinkage distributions, obtained from computations and experimental results [25], are shown in Figure 4.8. Again, a good agreement was found between predictions and experiments. From the results obtained in Cases One and Two, it was concluded that the developed finite element program can be used for thermal analysis of sand casting design.

4.3 Case Three - Low Pressure Die Casting of Aluminum Alloy Wheel

The third case is an aluminum alloy low pressure die casting. Ohtsuka et al. [62] analyzed the aluminum low pressure die casting by an explicit finite difference method. In his work computational results were compared with experimental data. The cross section of the aluminum wheel casting is shown in Figure 4.9, including initial conditions for temperature and locations for temperature measurements. The casting alloy was Al356 (AlSi7Mg) with the solidus temperature, 572°C and liquidus temperature, 610°C. The mold
Figure 4.7. Comparison of temperature history at four measuring points (see Fig. 4.5 for locations).
PREDICTED AND OBSERVED REGIONS OF MACROSHRINKAGE AND POROSITY

Figure 4.8. Comparison of shrinkage for Case Two between computed F.E.M. prediction and experiment [25], (Shrinkage ratio = 4.08%).
Figure 4.9. Cross section of low pressure aluminum wheel die casting (Case Three) (Positions 1-6 represent the locations for temperature measurements in [62]).
material was tool steel. The thermal properties for the casting and the molds, used in the simulation, are given in Table 4.6.

One important issue for this analysis is the thermal resistance between the casting and the metal mold. The mold was covered by a coating to improve fluidity and to protect the mold. Therefore, the thermal resistance at the metal-mold interface will be a function of coating thickness and coating type. Papai and Mobley [30] have summarized the heat transfer coefficients (the inverse of the thermal resistance) at the interface for solidifying systems. In the present simulation, the thermal resistance value of 100 cm² sec °C/cal was assumed for the overall casting and the value of 50 was chosen for locations in the rim and the flange (see Figure 4.10 for details). A mesh of 260 and 607 quadrilateral elements in casting and mold, respectively, was used for the finite element simulation.

Table 4.6 Thermal properties of steel and aluminum alloy for Case Three

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Thermal Conductivity (Kcal/m hr°C)</th>
<th>Heat Capacity (Kcal/Kg °C)</th>
<th>Density (Kg/m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aluminum Alloy</td>
<td>122</td>
<td>0.25</td>
<td>2400 (liquid)</td>
</tr>
<tr>
<td>mold steel</td>
<td>25.2</td>
<td>0.12</td>
<td>7750</td>
</tr>
<tr>
<td>Latent heat of Al356</td>
<td></td>
<td></td>
<td>93 Kcal/Kg</td>
</tr>
<tr>
<td>Liquidus and solidus temps</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Liquidus</td>
<td></td>
<td></td>
<td>610 °C</td>
</tr>
<tr>
<td>Solidus</td>
<td></td>
<td></td>
<td>572 °C</td>
</tr>
</tbody>
</table>
The heat loss in Al356 during the filling stage was considered by assuming an appropriate initial temperature distribution. The initial temperature distribution was taken from reference [62]. The initial temperatures were 710 °C in the region away from the boundary of the spoke and 620 °C outside the upper flange. The initial temperatures of the mold were assumed to be 400 °C at the stalk and 200 °C at the outside wall [62] (see Figure 4.10).

Figure 4.11(a), 4.11(b), and 4.11(c) show the calculated temperature distributions in the casting at 30, 45, and 300 seconds after solidification starts. The calculated temperatures in the steel mold at 300 seconds after solidification starts are shown in Figure 4.12. In the early stage of the solidification as shown in Figure 4.11(a), the upper flange was just about to solidify. At 300 seconds most of the casting was solidified as shown in Figure 4.11(c). Moreover, one can find that in Figure 4.11(b), there is a very wide range of mushy zone at the rim and the upper flange. This information can be correlated with the formation of shrinkage observed in experiments [62]. Since a large portion of the rim solidifies within a very short period of time, it is likely to have a centerline porosity formation in this area, which was observed in experiments [62]. The comparison of the experimental and computational solidification time at six locations (for locations see Figure 4.9) is shown in Table 4.7. From this table, it can be construed that the current finite element program can also be utilized for conducting thermal studies in low pressure die casting under the present working conditions.
Figure 4.10. Initial temperature distribution and thermal resistance conditions (After reference [62]).
Figure 4.11(a). Temperature distribution in the casting for Case Three at time = 30 seconds with temperature interval = 10 °C; liquidus temperature = 610 °C; and solidus temperature = 572 °C.
continued Figure 4.11

Figure 4.11(b). Temperature distribution in the casting for Case Three at time = 45 seconds with temperature interval = 10 °C; liquidus temperature = 610 °C; and solidus temperature = 572 °C.
continued Figure 4.11

TEMPERATURE INTERVAL = 10 °C

Figure 4.11(c). Temperature distribution in the casting for Case Three at time = 300 seconds with temperature interval = 10 °C; liquidus temperature = 610 °C; and solidus temperature = 572 °C.
Figure 4.12. Temperature distribution in the steel mold for Case Three at time = 300 seconds with temperature interval = 25 °C; liquidus temperature = 610 °C; and solidus temperature = 572 °C.
Table 4.7. Experimental and calculated solidification time in seconds.

<table>
<thead>
<tr>
<th>Position</th>
<th>Experiment</th>
<th>Calculation(present)</th>
<th>Calculation(Ohtsuka)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>34</td>
<td>32</td>
<td>34</td>
</tr>
<tr>
<td>2</td>
<td>36</td>
<td>45</td>
<td>42</td>
</tr>
<tr>
<td>3</td>
<td>65</td>
<td>85</td>
<td>76</td>
</tr>
<tr>
<td>4</td>
<td>90</td>
<td>115</td>
<td>106</td>
</tr>
<tr>
<td>5</td>
<td>214</td>
<td>265</td>
<td>269</td>
</tr>
<tr>
<td>6</td>
<td>45</td>
<td>48</td>
<td>46</td>
</tr>
</tbody>
</table>
The parameter, $G/\sqrt{R}$, was calculated at each node in all three cases discussed above. This parameter was used to predict the porosity for steel alloy castings. As discussed in chapter three, if the parameter is less than one (this value should be determined by correlation with the experimental observations for each alloy), then porosity is likely to occur. The result for Case Two is shown in Figure 4.13. Although the results of Case One are not shown here, all the nodes had a parameter greater than one. Thus, no porosity was predicted as reported in experiments [24]. For Case Two, one can find the zone where the predicted value of $G/\sqrt{R}$ is less than one. In experiments, the porosity zone was observed as shown in Figure 4.8. By comparing these two figures (4.8 and 4.13), it was found that the present calculation provided an introductory guidance in predicting the porosity by checking out the zone where $G/\sqrt{R}$ is less than one and the location which solidified last. Since the casting was made by an aluminum alloy for Case Three, there was no available criterion to decide whether or not porosity will occur. For this reason, the computed value of $G/\sqrt{R}$ was not correlated with the experimental results in this case.
Figure 4.13. Calculated $G/\sqrt{R}$ for Case Two (Cross-hatched represents the zone where $G/\sqrt{R} < 1$). The dimension of $G/\sqrt{R}$ is in $(\text{deg min})^{1/2}/\text{cm}$. 
4.4 Case Four - Evaluation of Heat Transfer Coefficient for a Steel Mold Aluminum Casting

In this section, the interface heat transfer coefficient will be determined by minimizing the errors between the calculated and measured temperatures. As mentioned in Case Three, the heat transfer coefficient in the mold/casting interface is the controlling factor to determine the solidification rate. The heat transfer coefficients can vary by several orders of magnitude depending on the type of materials at the interface, the thickness of casting and the coarseness of interface. Generally speaking, thinner casting sections have higher heat transfer coefficients. Also, metal molds have higher heat transfer coefficients than sand or ceramic molds [30]. In 1976, Sully [31] suggested that the heat transfer coefficients are time dependent. The heat transfer coefficient usually rises rapidly to a peak value and then gradually drops to a constant value. Ho and Pehlke [32,33] have found that both radiation and conduction exist at the interface once the gap formed. Morgan et al. [34] stated that the heat transfer coefficient is a function of location as well as time. Zeng and Pehlke [35] used the thickness of gap obtained from experiment to predict heat transfer coefficients. Hao et al. [36] solved the heat transfer coefficients by minimizing the square mean error between the calculated and measured temperatures from thermocouples. The techniques to solve the nonlinear inverse heat conduction problem were introduced by Beck [37]. The sum of the square function can be expressed as,

\[ f(h) = \sum_{i=1}^{N} \sum_{j=1}^{M} (T_i^c(h) - T_i^e)^2 \]  

(4-1)

where subscripts c and e refer to calculated temperatures and experimental temperatures, respectively, and superscripts i and j denote location i and time
step j. $M$ is the total number of time steps and $N$ is the total number of measurements.

An axisymmetric aluminum alloy casting with steel mold was investigated in [63]. The height of the casting was 160 millimeters and the radius was 60 millimeters. The thickness of the die was 30 millimeters. A layer of glass wool mat with thickness 10 millimeters was placed on the top of casting and die as an insulator. Four thermocouples were used in the experiment for temperature measurements. Thermocouples A and B were located, respectively, at 1.6 mm away from the center and 6 mm away from interface between the die and the casting. Thermocouples C and D were placed at 2 and 5 mm from the casting and the die interface, respectively. The configuration of the experiment and locations of measurement can be found in Figure 4.14.

The thermal properties of the casting alloy and the mold are listed as follows,

**Aluminum alloy:**

- **Solidus temperature:** 645 °C  
- **Liquidus temperature:** 657 °C  
- **Thermal Conductivity:** 122 Kcal/m hr °C  
- **Heat Capacity:** 0.25 Kcal/Kg °C  
- **Density:** 2700 Kg/m$^3$  
- **Latent heat:** 93 Kcal/Kg  

**Mold steel (H13):**

- **Thermal Conductivity:** 25.2 Kcal/m hr °C  
- **Heat Capacity:** 0.12 Kcal/Kg °C  
- **Density:** 7750 Kg/m$^3$
Figure 4.14. Configuration of the experiment and locations of measurement.
The heat transfer coefficients at the interface were determined by minimizing the difference between the calculated and measured temperatures at four locations, A, B, C, and D. The error function used in this analysis was,

$$\text{Error} = \left| T_c^A - T_e^A \right| + \left| T_c^B - T_e^B \right| + \left| T_c^C - T_e^C \right| + \left| T_c^D - T_e^D \right|$$

(4-2)

where subscript c means the calculated temperature, subscript e means the experimental temperature and superscripts A, B, C, and D denote the temperatures of thermocouples at A, B, C, and D. Since the temperature was recorded for every five seconds in experiments, different h values were used to calculate temperatures for each period of five seconds. The h value producing the minimum error was chosen as the calculated heat transfer coefficient. The time step used in the finite element analysis was one second. Besides this procedure, the following time dependent heat transfer coefficient was used in the simulation as,

$$h = 814. / (\text{time(seconds)} \times 0.025 + 1).$$

(4-3)

in cal/m$^2$ sec °C. Figure 4.15 shows the heat transfer coefficients from Equations (4-2) and (4-3) versus time(sec). One can find the heat transfer coefficients obtained from Equation (4-3) are very close to the evaluated values when the elapsed time is larger than 100 seconds. The heat transfer coefficient at the glass mat was assumed to be 40.7 cal/m$^2$ sec °C. The product of the Stefan Boltzmann constant and the emissivity at the external surface of the mold was $7.74 \times 10^{-8}$ cal/m$^2$ sec °C$^4$.

The mesh used in the simulation consisted of 480 and 840 quadrilateral elements in the casting and in the mold, respectively. Figure 4.16 shows the predicted temperature distributions by minimizing Equation (4-2) compared to experimental results at four locations [63]. It is seen from Figure 4.16 that
Figure 4.15. Calculated heat transfer coefficients by minimizing Equation (4-2) and assumed heat transfer coefficients by Equation (4-3). (Unit is cal/m² sec °C).
Figure 4.16. Comparison between predicted and experimental temperatures. Predicted values were calculated by minimizing Equation (4-2).
the predicted heat transfer coefficients used in computations reproduce
temperature versus time accurately for locations B, C, and D. However, the
present scheme fails to predict the time of complete solidification for location
A. This error might be reduced by changing the minimizing scheme to
determine the heat transfer coefficient and by introducing the different heat
transfer coefficients at different locations.

Figure 4.17 shows comparison between the predicted temperatures by
Equation (4-3) and the experimental results. One can find that this heat
transfer coefficient generates more accurate temperature predictions for
location A. However, a larger discrepancy has been found in the temperature
distributions for locations C and D. Besides, the temperature reduction in the
computed temperature for location A is more rapid than that in the
experiment. This may be due to the use of the temperature recovery method
since the temperature predicted by this method has been observed to have a
larger thermal gradient than the analytic solution for solidification of pure
metals (See Chapter 6).

In conclusion, the proposed technique can be a useful scheme to
evaluate the interface heat transfer coefficients for different locations and
time. However, further work needs to be done to get more accurate
predictions for the location far from the interface.
Figure 4.17. Comparison between predicted and experimental temperatures. Predicted values were calculated by using Equation (4-3).
CHAPTER V
FINITE ELEMENT MODELING OF MOMENTUM,
HEAT AND SPECIES TRANSPORT

A two-dimensional finite element model was demonstrated to solve casting processes in an earlier chapter. In this chapter, a general solidification model, including natural convection, interdendritic flow, and species transport is discussed. A literature survey which includes various numerical and experimental work is presented in section 5.1. Then, the solidification for pure metals in the presence of natural convection in the liquid pool is solved by the front tracking method [13] and numerical results are shown in section 5.2. The computed temperature distributions are compared with the experimental results and the agreement was reasonably accurate. A technique to solve the solidification problems with a moving boundary is introduced in section 5.3. This technique will calculate the position of the phase front by the temperature recovery method such that a general two-dimensional solidification problem can be solved. Numerical results by the front tracking method and temperature recovery method will be compared to each other. In Section 5.4, the solidification of a binary alloy is described. The effect of interdendritic flow by using Darcy's law and species transport was included. The finite element formulation of these equations is also made and some problem-solving techniques are discussed.
5.1 Literature Survey

On the topic of the solidification of a pure material in the presence of convective heat transfer, much research work has been conducted by using finite difference and finite element methods. Implicit finite difference method has been used by Sparrow, Patankar, and Ramadyani [64]. In 1982, Ramachandran et al. [39] presented a two-dimensional numerical model of solidification with heat and momentum transport. They solved coupled momentum and heat transport equations with the aid of Alternating Direction Implicit finite difference method. They found that fine grids are necessary for high Rayleigh number (\(Ra>10^5\)) to accommodate a large velocity gradient in the fluid near the phase interface. Wolff and Viskanta [44] also used a finite difference method to solve the solidification of a pure metal in a rectangular cavity in the presence of superheat in liquid and natural convection. In their work, experiments of solidification of tin were performed and the computed and experimental results were compared with each other. The agreement between measured and predicted results was good for temperature while it was just fair in predicting the position of the interface. Experimental data such as temperature and phase front of a solidifying gallium system [43] have been obtained so that computed results can be compared with them.

Murthy et al. [40] investigated the interaction between the solute concentration, temperature and velocity by using the SIMPLER algorithm [65]. In the same case, they computed the flow and heat transfer for high Rayleigh number (\(Ra=10^6\)). Hibbert et al. [66] introduced a mathematical model to predict the transient solidification in a cooled pipe with flow at low Reynolds
number (585 to 1617). The enthalpy formulation was used to include the release of latent heat and the coupled flow and heat equations were solved by the finite difference method in this work.

Some research work using the finite element method can also be found in the literature. Gartling [41] performed a finite element analysis of convective heat transfer with phase change. The effective capacity technique was adopted to handle the release of latent heat and the fictitious viscosity was applied to the solid region. The analysis included solidification within a cooled pipe and solidification in a cylinder in the presence of natural convection. Voller et al. [1] used the enthalpy method to solve solidification with convection. Desai et al. [42] simulated forced and natural convection during the filling stage in a sand casting. A continuous deforming finite element method was used to solve the effect of forced convection in filling. Hsu and Rubinsky [67] used a quasi-stationary finite element model to study the fluid flow and heat transfer within the melt of plasma.

Recently, some progress has been made in solving solidification problems with momentum, heat and species transport in solidifying alloy systems. The main difference involved in the simulation of alloys is the presence of a mushy zone and species transport. The interdendritic flow can be assumed as a Darcy's flow introducing permeability as a function of liquid fraction. Detailed investigation about this relation will be provided in Section 5.4. Using this approximation, Beckermann and Viskanta [48] solved the phase change problem in a porous media including natural convection. They also performed experiments in a square enclosure to check their numerical results from the finite difference method. The material used in the experiment was gallium as fluid and glass bead as the porous matrix. The
permeability used in the analysis was calculated from the Kozeny-Carman equation. Ohnaka et al. [49] studied fluid flow for the casting of steel ingots using the direct finite difference method. They found that the downward thermal convection flow increased as the height of ingot increased. They also concluded that the presence of fluid flow tends to reduce thermal gradients in the liquid region such that equiaxed structure is likely to form. Voller et al. [46,47] have set up some fixed grid techniques to solve the convection-diffusion in a mushy region for phase change problems. They adopted the enthalpy method to deal with latent heat and set an artificial permeability (very large) in the solid region. Good agreement was obtained for the position of the melting phase front between their computed results and experimental data[47].

Bennon and Incropera [50] introduced a continuum model for momentum, heat and species transport for a binary alloy system. The equations were solved by implicit control volume-based finite-difference scheme (SIMPLER)[65]. The upwinding technique was applied on the advection-diffusion terms [38]. The solidification of an aqueous solution of ammonium chloride (NH$_4$Cl-H$_2$O) in a rectangular cavity was solved by Bennon at al. [45,51]. They found that computed results showed some irregularity in interfacial surface. Experimental data were also obtained and compared with numerical results by Christenson and Incropera [52,53]. The comparison included temperature and composition distributions at several locations and the positions of liquidus and solidus at different times. The agreement was found to be fair.
5.2 Solidification with Natural Convection by Front Tracking Method

Fluid flow induced by natural convection occurs in many solidification processes. This kind of fluid flow can influence the shape of the liquid-solid interface and temperature distribution in the casting metal. As discussed in the literature survey, several papers analyzed the natural convection effect using various techniques such as finite element and finite difference methods. In this section, the front tracking method was used to solve the solidification of pure metal including natural convection.

The description of the problem will be introduced as follows. Solidification with the natural convection effect will be considered in the two-dimensional domain $D = \Omega_1(t) \cup \Omega_2(t)$ (Figure 5.1). Domains $\Omega_1(t)$ and $\Omega_2(t)$ are time dependent and represent the solid and liquid phases, respectively. $\Gamma_1(t)$ and $\Gamma_2(t)$ denote the fixed boundary of solid and liquid. $\epsilon(t)$ denotes the solid/liquid moving boundary.

The following physical assumptions are made in the modeling of the problem:

1. **Boussinesq approximation**: The physical properties of the solid and liquid are assumed to be constant except for the density difference due to temperature variation and composition in the liquid. The flow motion results from the buoyancy forces, which are solely caused by the density difference in the liquid.

2. The flow developed in the liquid is assumed to be laminar.

3. The liquid is assumed to be Newtonian with negligible viscous energy dissipation.

The mathematical expression of the Boussinesq approximation is,

$$\rho = \rho_0[1 - \beta_\tau(T - T_\epsilon) - \beta_c(c^s - c^l_\epsilon)].$$  \hspace{1cm} (5-1)
Figure 5.1. Schematic of solid-liquid interface in a solidifying system.

where \( \beta_T \) is thermal expansion coefficient, \( \beta_c \) is solutal expansion coefficient, \( T_e \) is eutectic temperature, \( f^a_l \) is composition of constituent \( a \) in liquid phase, \( f^a_{l,e} \) is eutectic composition of constituent \( a \) in liquid phase and \( \rho_0 \) is material density at eutectic temperature and composition. The body force due to the Boussinesq assumption can be expressed as,

\[
F_y = g[\beta_T(T - T_e) + \beta_c(f^a_l - f^a_{l,e})].
\]

(5-2)

Then, from the discussion of Appendix D, the conservation equation of energy, equation (D-19), for the solid domain is,

\[
\frac{\partial}{\partial t}(\rho_c c_s T) = \nabla \cdot (k_s \nabla T).
\]

(5-3)

The energy conservation equation in the liquid phase can be expressed as follows;

\[
\frac{\partial}{\partial t}(\rho_l c_l T) + \nabla \cdot (\rho_l c_l \nabla T) = \nabla \cdot (k_l \nabla T).
\]

(5-4)

The relative motion in equation (D-23) will not appear because the domain \( \Omega_2 \) contains one phase and one material.
The continuity equation in the liquid phase is derived from equation (D-6) and with the assumption that the liquid density is constant as,

\[ \nabla \cdot \mathbf{V} = 0. \quad (5-5) \]

The momentum equations in the x and y directions in the liquid phase are from equations (D-16) and (D-17), respectively. Since the solidification of pure material is calculated in this section, no mushy zone will form. The term containing the permeability will vanish. The momentum equation in the x direction is,

\[ \frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{V} \mathbf{u}) = \nabla \cdot (\mu \nabla \mathbf{u}) - \frac{\partial p}{\partial x}. \quad (5-6) \]

By applying equation (5-2) to equation (D-17), we can find the momentum equation in the y direction as,

\[ \frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{V} \mathbf{v}) = \nabla \cdot (\mu \nabla \mathbf{v}) - \frac{\partial p}{\partial y} + \rho \beta \gamma (T - T_0). \quad (5-7) \]

Here, \( T_0 \) is the eutectic temperature. Only the temperature difference will contribute to the driving force since changes in concentration will not be present for the case of a pure metal.

In the boundary of the liquid and the phase interface \( (\Gamma_1(t) \cup \Gamma_2(t)) \), the kinematic no-slip condition is assumed to exist. The initial and boundary conditions are,

**Initial conditions**

at \( t = 0 \):
- \( T_1 = T_0 \), in \( \Omega_1(t) \)
- \( T_2 = T_0 \), in \( \Omega_2(t) \) \quad (5-8)

**Energy boundary condition**
\[ a_1(\nabla T_1) \cdot \vec{n}_1 + b_1 \theta_1 = c_1, \quad \text{on } \Gamma_1(t) \]
\[ a_2(\nabla T_2) \cdot \vec{n}_2 + b_2 \theta_2 = c_2, \quad \text{on } \Gamma_2(t) \]
\[ T_1 = T_2 = T_m, \quad \text{on } e(t) \quad (5-9) \]

**Velocity boundary condition**

\[ u = v = 0, \quad \text{on } \Gamma_2(t) \text{ and } e(t) \quad (5-10) \]

Next, the governing equations (5-3) to (5-7), and initial and boundary conditions, (5-8) to (5-10) for this problem are transformed into non-dimensionalized form. The non-dimensionalized variables are defined as follows,

\[ x^* = x / C_L, \quad y^* = y / C_L \]
\[ u^* = u C_L / \alpha_2, \quad v^* = v C_L / \alpha_2 \]
\[ \text{Ste} = c(T_i - T_m) / L, \quad \text{Ste}^* = \text{Ste} \frac{k_1}{k_2} \]
\[ R_a = \alpha_1 / \alpha_2, \quad R_k = k_1 / k_2 \]
\[ \text{Pr} = \nu / \alpha_2 = \mu / \rho_1 \alpha_2, \quad \text{Ra}_T = g \beta_T (T_i - T_m) C_L^3 / \nu \alpha_2 \]
\[ t^* = t \alpha_2 / C_L^2, \quad \theta = (T - T_m) / (T_i - T_m) \quad (5-11) \]
\[ P^*_d = p C_L^2 / \rho_1 \alpha_2^2 \]

where \( C_L \) is the characteristic length, \( L \) is the latent heat of diffusion and subscripts 1,2 represent the state of solid and liquid, respectively. \( \text{Ste} \), \( \text{Pr} \) and \( \text{Ra}_T \) represent the Stefan, Prandtl and Rayleigh number, respectively. \( T_i \) is the initial casting temperature and \( T_m \) is the solidus temperature.

The variables to be determined in this problem are the position of the moving interface, the temperature distribution in the solid and liquid, and the velocity distribution in the liquid. The governing equations for this problem are,

**Continuity**
\[ \frac{\partial u^*}{\partial x^*} + \frac{\partial v^*}{\partial y^*} = 0 \]  

(5-12)

\[ \begin{align*}  
& \frac{\partial u^*}{\partial t^*} + u^* \frac{\partial u^*}{\partial x^*} + v^* \frac{\partial u^*}{\partial y^*} = - \frac{\partial P^*}{\partial x^*} + \text{Pr} \nabla^* \cdot (\nabla^* u^*) \\
& \frac{\partial v^*}{\partial t^*} + u^* \frac{\partial v^*}{\partial x^*} + v^* \frac{\partial v^*}{\partial y^*} = - \frac{\partial P^*}{\partial y^*} + \text{Pr} \nabla^* \cdot (\nabla^* v^*) - \text{Pr Ra} \frac{f_2}{T} \theta_2 
\end{align*} \]

(5-13)

\begin{align*}
\text{Energy in liquid} \\
& \frac{\partial \theta_2}{\partial t^*} + u^* \frac{\partial \theta_2}{\partial x^*} + v^* \frac{\partial \theta_2}{\partial y^*} = \nabla^* \cdot (\nabla^* \theta_2) 
\end{align*}

(5-14)

\[ \frac{\partial \theta_1}{\partial t^*} = \text{Ra} \nabla^* \cdot (\nabla^* \theta_1) \]

(5-15)

\[ \frac{\partial \theta_1}{\partial n^*} - \text{Ra} \frac{\partial \theta_2}{\partial n^*} = \text{St} \nabla^* \cdot v^* \]

(5-16)

\begin{align*}
\text{Initial conditions} \\
& \text{at } t^* = 0; \quad \theta_1 = \theta_1^0, \text{ in } \Omega_1(t) \\
& \theta_2 = \theta_2^0, \text{ in } \Omega_2(t) 
\end{align*}

(5-17)

\begin{align*}
& a_1^* (\nabla^* \theta_1) \cdot \n^*_1 + b_1 \theta_1 = c_1^*, \quad \text{on } \Gamma_1(t) \\
& a_2^* (\nabla^* \theta_2) \cdot \n^*_2 + b_2 \theta_2 = c_2^*, \quad \text{on } \Gamma_2(t) \\
& \theta_1 = \theta_2 = 0, \quad \text{on } \varepsilon(t) 
\end{align*}

(5-18)

\begin{align*}
\text{Velocity boundary condition} \\
& u^* = v^* = 0, \quad \text{on } \Gamma_2(t) \text{ and } \varepsilon(t) 
\end{align*}

(5-19)

Here, \( \nabla^* = \frac{\partial}{\partial x^*} \mathbf{i} + \frac{\partial}{\partial y^*} \mathbf{j} \). \( v^*_n \) is the velocity at the phase front in the direction of the outward normal vector at the interface. \( \mathbf{V} = u^* \mathbf{i} + v^* \mathbf{j} \) and the
continuity equation are used in deriving Equation (5-13). Equation (5-16) shows the treatment of latent heat in the front tracking method.

Yoo [13] obtained the Galerkin formulation of Equation (5-16) in matrix form,

\[
\bar{A}_1 \bar{T}_1 - \bar{A}_2 \bar{T}_2 = \bar{L}_{ph} \frac{d\bar{s}}{dt^*} \tag{5-20}
\]

where \(\bar{T}_1\) and \(\bar{T}_2\) are the dimensionless temperature vectors and \(\bar{s}\) is position vector of the interface and,

\[
\bar{A}_1 = \sum_m \int_{e(t)} \bar{U}^{(m)(o)} \bar{B}_1^{(m)(o)} dS \\
\bar{A}_2 = \sum_m \int_{e(t)} R_k^{-1} \bar{U}^{(m)(o)} \bar{B}_2^{(m)(o)} dS \\
\bar{L}_{ph} = \sum_m \int_{e(t)} S \bar{t} e^{-1} \bar{U}^{(m)(o)} \bar{U}^{(m)(o)} dS \tag{5-21}
\]

where \(m\) represents number of elements near the solid/liquid interface and \(\bar{U}^{(o)}\) is the surface interpolation matrix defined as,

\[
\bar{U}^{(o)} = \begin{bmatrix} 
\frac{1}{2} (1 + r) & 0 & \frac{1}{2} (1 - r) & 0 \\
0 & \frac{1}{2} (1 + r) & 0 & \frac{1}{2} (1 - r)
\end{bmatrix} \tag{5-22}
\]

and \(\bar{B}_1^{(o)}\) matrix is defined as,

\[
\bar{B}_1^{(o)} = \frac{1}{4} \bar{J}^{(o)-1} \begin{bmatrix} 
2 & -2 & 0 & 0 \\
(1 + r) & (1 - r) & -(1 - r) & -(1 + r)
\end{bmatrix} \tag{5-23}
\]

Here, \(r\) is the local coordinate in a two-element domain at the interface (Figure 5-2) and \(\bar{J}^{(o)}\) is the Jocobian matrix of the transformation from the \(x,y\) coordinate to \(r,s\) coordinate (Figure 5.2).

Equation (5-20) is a finite element formulation of the energy balance on the solid-liquid interface. With this formulation, one can find the position of the new interface at each time step with the temperature distribution of solid
and liquid. The temperature of solid and liquid can be solved separately in its own domain. To obtain the finite element formulation of Equation (5-12) to (5-16), the unknown variable $\theta_1$ can be approximated over the domain $\Omega_1$ by a combination of interpolation functions:

$$\theta_1(\vec{x}, t) = \sum_q T_q(t) N_q(\vec{x})$$  \hspace{1cm} (5-24)

where $q$ is the nodal point of the element, $T_q$ are the nodal non-dimensional temperature and $N_q(\vec{x})$ are interpolation functions. Similar forms for unknown variables $\theta_2$, $u^*$ and $v^*$ over the domain $\Omega_2$ can be obtained as:

$$\theta_2(\vec{x}, t) = \sum_q T_q(t) N_q(\vec{x})$$

$$u^*(\vec{x}, t) = \sum_q U_q(t) N_q(\vec{x})$$

$$v^*(\vec{x}, t) = \sum_q V_q(t) N_q(\vec{x})$$  \hspace{1cm} (5-25)

where $T_q$, $U_q$, and $V_q$ are the nodal non-dimensional temperatures and components of velocity, respectively and $N_q(\vec{x})$ are interpolation functions.

---

Figure 5.2 Schematic diagram of a two-element domain
In the solid domain, temperature distributions can be obtained by using the weak formulation of Equation (5-15). Since there is no liquid motion in the solid, the finite element formulation of the energy conservation equation in solid is similar to Equation (2-1). One can solve this equation by similar technique described in chapter 2.

The weak formulations of Equations (5-12) through (5-14) are much more difficult to solve. The difficulties result from the nonlinear terms in the velocity component in Equation (5-13) and the coupling terms of Equation (5-13) and (5-14). To satisfy the continuity of velocity component (Equation (5-12)), the penalty method was used by,

$$ P^*_j = -\lambda \frac{\partial u^*_j}{\partial x^*_j} \quad (5-26) $$

where $\lambda$ is the penalty coefficient. The penalty coefficient has a range of $10^5$ to $10^7$. In this analysis, the penalty coefficient used was $10^6$.

To solve the coupled Equations (5-13) and (5-14), the following numerical techniques were used,

1. The $u^*_j$ term from $u^*_j \frac{\partial u^*_i}{\partial x^*_j}$ in Equation (5-13) was linearized by using the value from the previous iteration, $^{i-1}u^*_j$.

2. The temperature and velocities were coupled only by the buoyancy term ($Pr Ra f_1 \dot{\theta}_2$ in Equation (5-13)). They can be decoupled if the temperatures from the buoyancy term are replaced with the temperatures from the previous iteration, $^{i-1}T_2 + \Delta t'$.

3. The modified Newton-Raphson iteration procedure was used.

4. The implicit time discretization was used.
Then, the matrix form of the weak formulation of Equations (5-13) and (5-14) was shown as follows:

\[
\frac{1}{\Delta t_1} [M M]^t + \Delta t^t \begin{bmatrix} U^t + \Delta t^t - U^t \nonumber \\
V^t + \Delta t^t - V^t \nonumber \end{bmatrix} + [\bar{\mathcal{C}} + \text{Pr} \bar{K} \bar{L}] + \Delta t^t \begin{bmatrix} U^t + \Delta t^t \\
V^t + \Delta t^t \nonumber \end{bmatrix} 
\]

\[
= \begin{bmatrix} \bar{R}_1 \\
\bar{R}_2 \nonumber \end{bmatrix} + \text{Pr} \text{Ra}_T \bar{B} M \begin{bmatrix} -1 \bar{T}_2 + \Delta t^t \nonumber \\
-1 \bar{T}_2 + \Delta t^t \nonumber \end{bmatrix} + \text{Pr}^{-1} \bar{K}_2 \begin{bmatrix} -1 \bar{T}_2 + \Delta t^t \nonumber \\
-1 \bar{T}_2 + \Delta t^t \nonumber \end{bmatrix} 
\]

(5-27)

\[
\frac{1}{\Delta t_1^2} \bar{M}_2 \begin{bmatrix} t^t + \Delta t^t - \bar{T}_2 + \Delta t^t \nonumber \\
\bar{T}_2 + \Delta t^t \nonumber \end{bmatrix} + (\bar{C}_{11} + \bar{C}_{22}) + \bar{C}_{11} + \Delta t^t \begin{bmatrix} t^t + \Delta t^t \\
\bar{T}_2 + \Delta t^t \nonumber \end{bmatrix} 
\]

+ \bar{K}_2 \begin{bmatrix} \bar{T}_2 + \Delta t^t \\
\bar{T}_2 + \Delta t^t \nonumber \end{bmatrix} = \bar{Q}_2
\]

(5-28)

where,

\[
[M M] = \begin{bmatrix} M_2 & 0 \\
0 & M_2 \nonumber \end{bmatrix}, \quad [B M] = \begin{bmatrix} 0 \\
0 \nonumber \end{bmatrix} 
\]

\[
[\bar{C}] = \begin{bmatrix} \bar{C}_{11} + \bar{C}_{22} & 0 \\
0 & \bar{C}_{11} + \bar{C}_{22} \nonumber \end{bmatrix} 
\]

\[
[K] = \begin{bmatrix} 2\bar{K}_{11} + \bar{K}_{22} & \bar{K}_{12} \\
\bar{K}_{12}^T & \bar{K}_{11} + 2\bar{K}_{22} \nonumber \end{bmatrix} 
\]

\[
[L]\quad \begin{bmatrix} L_{11} & L_{12} \\
L_{12}^T & L_{22} \nonumber \end{bmatrix} 
\]

\[
\bar{M}_2 = \sum_m \int_{\Omega_j^{(m)}} \bar{N}^{(m)} \bar{N}^{(m)} d\Omega 
\]

\[
\bar{C}_{11} = \sum_m \int_{\Omega_j^{(m)}} -1 \bar{u} \bar{N}^{(m)} B_1^{(m)} d\Omega 
\]

\[
\bar{C}_{22} = \sum_m \int_{\Omega_j^{(m)}} -1 \bar{v} \bar{N}^{(m)} B_2^{(m)} d\Omega 
\]
Here, $N^{(m)}$ and $N^{s(m)}$ are the shape functions of 2-D four-node element and 1-D linear element, respectively. $B_1^{(m)}$ and $B_2^{(m)}$ are the spatial gradient matrix in x and y directions. $n_{2x}$ and $n_{2y}$ are the components of the unit outward vector at the boundary of liquid in the x and y directions, respectively.

The calculation procedure to solve Equations (5-27) and (5-28) was, first, to calculate the velocity from the weak formulation of Equation (5-27). Then, the energy balance equation was solved to determine the temperature distribution. The weak formulations of Equation (5-27) and (5-28) were continuously iterated until the velocity and temperature fields converged to a given value.

Once the temperature and velocity distributions were determined in the liquid domain, Equation (5-20) was solved in an area near the solid/liquid interface and a new interfacial position was determined. In summary, the whole procedure to apply the front tracking method is as follows,

(1) At the beginning of each time step, a new mesh for liquid and solid domain will be created since a new interfacial position was obtained (by solving Equation (5-20) from last time step). Since the node positions of
the new mesh are different from those of the old mesh, the temperatures and velocity of the new mesh were extrapolated from the temperature and velocity of the old mesh.

(2) The temperature distribution in the solid domain was calculated by solving Equation (5-15).

(3) The temperature and velocity distribution in the liquid domain was determined by solving Equations (5-27) and (5-28). The numerical techniques used have been discussed above.

(4) By using the temperature distribution in solid and liquid, Equation (5-20) can be solved and the new interfacial position can be determined. All the steps above can be moved to the next time step until simulation is completed.

In the following part of this section, an aluminum casting with square enclosure was considered including the natural convection effect. It was assumed that a prescribed temperature was imposed on one of the vertical walls while adiabatic boundary conditions were imposed on the other walls (See Figure 5.3). The thermal properties of aluminum are listed in Table 5.1. Several dimensionless parameters for aluminum are given in Table 5.2. The characteristic length was 50 cm. The initial temperature was 710 °C while the prescribed temperature at the left wall was 510 °C. A mesh with 20 x 20 element was used and the time step was 6.84 second.

The velocity and temperature distributions for Rayleigh number = 100,000 are shown in Figures 5.4(a), (b) and Figures 5.5(a), (b), respectively. Similar results for Rayleigh number=10,000 are in Figure 5.6 and Figure 5.7 at time=512 seconds. Figures 5.4(a) and 5.5(a) represent the early stage of solidification (t=171 seconds) while Figures 5.4(b) and 5.5(b) represent the later
Table 5.1. Thermal properties of aluminum

<table>
<thead>
<tr>
<th></th>
<th>Solid</th>
<th>Liquid</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k$</td>
<td>0.597</td>
<td>0.239</td>
<td>cal/cms °C</td>
</tr>
<tr>
<td>$c$</td>
<td>0.215</td>
<td>0.259</td>
<td>cal/g °C</td>
</tr>
<tr>
<td>$L$</td>
<td>95.0</td>
<td>95.0</td>
<td>cal/g</td>
</tr>
<tr>
<td>$T_m$</td>
<td>660</td>
<td>660</td>
<td>°C</td>
</tr>
<tr>
<td>$\alpha_2$</td>
<td>1.102</td>
<td>0.3662</td>
<td>cm$^2$/s</td>
</tr>
</tbody>
</table>

Table 5.2. Dimensionless parameters for aluminum

<table>
<thead>
<tr>
<th>Group</th>
<th>Definition</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rayleigh number</td>
<td>$Ra = \beta g (T_1 - T_m) C_L^3 / \alpha_2 \nu$</td>
<td>$10^4, 10^5$</td>
</tr>
<tr>
<td>Prandtl number</td>
<td>$Pr = \nu / \alpha_2$</td>
<td>0.03041</td>
</tr>
<tr>
<td>Stefan number (solid)</td>
<td>$Ste_1 = c_1 (T_1 - T_m) / L$</td>
<td>0.1131</td>
</tr>
<tr>
<td>Ratio</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Conductivity</td>
<td>$R_k = k_1 / k_2$</td>
<td>2.4979</td>
</tr>
<tr>
<td>Thermal diffusivity</td>
<td>$R_\alpha = \alpha_1 / \alpha_2$</td>
<td>3.0093</td>
</tr>
</tbody>
</table>
Figure 5.3 Dimensions and Boundary Conditions for Solidification with Natural Convection Effect
Figure 5.4(a). Vector plot of the velocity field for $Ra_x = 10^5$ at time = 171 seconds.
continued Figure 5.4

Figure 5.4(b). Vector plot of the velocity field for $Ra=10^5$ at time = 512 seconds.
Figure 5.5(a). Temperature distribution for $Ra_t = 10^5$ at time = 171 seconds with the temperature interval = 5 °C.
Figure 5.5(b). Temperature distribution for $Ra = 10^5$ at time = 512 seconds with the temperature interval = 5 °C.
Figure 5.6. Velocity vector field for $Ra_t=10,000$ at time $= 512$ seconds.
Figure 5.7. Temperature distribution for $Ra_T=10,000$ at time = 512 seconds with the temperature interval = 5 °C.
stage of solidification (t=512 seconds). Comparing the velocity field in Figure 5.4(b) and Figure 5.6, one can find the velocities from Ra=10^5 are larger than those from Ra=10^4. This means that the Rayleigh number is a decisive parameter, influencing the magnitude of natural convection and location of the phase front. From Figures 5.5(b) and 5.7, one can also observe that the natural convection has a significant effect on the temperature distribution. Figure 5.8 shows the phase front at 512 seconds, for Ra_x=10^4, and 10^5. For Ra_x=10^4 the phase front is nearly flat while for Ra_x=10^5 it is curved. These results show that convection has a significant effect on the shape of solid/liquid interface, resulting in different grain boundary. The analysis of solidification with natural convection is expected to provide a more accurate microstructure prediction than the analyses without convection.

The analytical solution for the one-dimensional Stefan problem without convection can be easily obtained in [68-70]. In Figure 5.9, the computed temperature distributions along the x axis by the front tracking method (time step used was 6.84 second) and by the temperature recovery method (time steps used were 6.84 and 1.368 second) were compared with the analytical result. As claimed by Yoo et al. [12], the front tracking method provides accurate prediction of the location of the phase front for the solidification of pure material with less computation time. The temperature recovery method can provide accurate predictions for temperature if a smaller time step (1.368 second) is used.

In addition, the calculated solidification results from the front tracking method with natural convection effect were compared with the experimental data obtained by Gau and Viskanta [43]. They chose gallium because of its low melting temperature and its material properties which are well documented
Figure 5.8. Solid/liquid interfaces for different Rayleigh numbers at time
= 512 seconds.
Figure 5.9. Temperature distributions along the x axis at 171 seconds without the natural convection effect.
in the literature [71,72]. The main drawback to use this metal was that the conductivity and coefficient of thermal expansion are anisotropic. The thermal conductivity varies from 33.49 W/m/°K along crystal axes to 40.82 W/m/°K along a axis and 88.47 W/m/°K along b axis. The material properties used in the analysis were assumed to be constant as follows:

<table>
<thead>
<tr>
<th>Property</th>
<th>Liquid</th>
<th>Solid</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_p$ (J/kg/°K)</td>
<td>397.6</td>
<td>372.3</td>
</tr>
<tr>
<td>$k$ (W/m/°K)</td>
<td>33.49</td>
<td>40.82</td>
</tr>
<tr>
<td>$\rho$ (kg/m$^3$)</td>
<td>6.0947</td>
<td>5.9037</td>
</tr>
<tr>
<td>$\alpha$ (m$^2$/s)</td>
<td>1.382</td>
<td>1.857</td>
</tr>
<tr>
<td>$L$ (kJ/kg)</td>
<td>80.16</td>
<td>80.16</td>
</tr>
<tr>
<td>$T_m$ (°C)</td>
<td>29.78</td>
<td>29.78</td>
</tr>
</tbody>
</table>

The definitions of Rayleigh number ($Ra_T$), Stefan number ($Ste$) and Prandtl number ($Pr$) were described in Table 5.2. The values of these three constants were obtained from Beckmann et al. [48] who solved natural convection and phase change in a porous media. The values used in this simulation are,

$$Ra_T = 1.1503 \times 10^5$$
$$Ste = 0.0993$$
$$Pr = 0.0208.$$ 

Both the initial temperature and hot wall temperature were 34°C and the temperature of the cold wall was 12.5°C. The width of the rectangular enclosure was 8.89 cm while the height was 4.445 cm. The hot and cold walls are located at the right and the left side of the enclosure.
For the front tracking method, a $20 \times 20$ mesh was used in the simulation. The mesh deformed constantly according to the changes in shape of the phase front. The time step used in analysis was 0.572 sec. The convergence of velocity calculation became more difficult to obtain as the convection flow increased. The simulation stopped after about 3 minutes due to the limitation of computational time and convergence of velocity calculation. The cost of CPU in CRAY X-MP/28 was about 13 minutes. Since the implicit time discretization was used, most CPU time (70%) was spent in triangulizing the matrix.

The computed and measured temperatures [43] along the half height two minutes after solidification started are shown in Figure 5.10. There was good agreement between predictions and measurements of temperatures. Because of the fluid flow in the region of liquid metal, the temperatures are uniformly distributed except in the neighborhood of the hot wall. This uniformity of liquid temperature has been observed by other authors [49]. The temperature distributions and the velocity vector plot at times = 0.238 min and 2.33 min are shown in Figure 5.11 and Figure 5.12 respectively. At 0.238 minutes, the gravity induced velocity is distributed near the interface and thermal gradient at this region is very high. The bend of isothermal line results from the effect of natural convection, that is, hotter liquid moved upward while cooler liquid will moved downward. At 2.33 minutes, the magnitude of the velocity becomes larger and the center of vorticity is close to the center of liquid zone. The velocity was not just distributed near the interface but in the whole liquid domain. In the middle part of the liquid, the isothermal lines are aligned horizontally while at the two ends, the isotherms
Figure 5.10. Geometry and temperature distributions along the half height at 2 minutes after solidification starts with $T_1=34^\circ C$, $T_h=34^\circ C$, and $T_c=12.5^\circ C$. 
Figure 5.11. Velocity vector and temperature distribution at 0.238 minutes after solidification starts with \( T_i=34^\circ C, T_h=34^\circ C, \) and \( T_c=12.5^\circ C. \)
Figure 5.12. Velocity vector and temperature distribution at 2.33 minutes after solidification starts with $T_i=34^\circ C$, $T_h=34^\circ C$, and $T_c=12.5^\circ C$. 
are still aligned vertically. If we trace the temperature along the half height, we can find the temperature is practically constant for a very large region of liquid, which can also be observed in Figure 5.10. With the results of Figures 5.10 through 12, the front tracking method can predict reasonably accurate temperature distributions for a solidifying system of a pure metal with natural convection effect.
5.3 Solidification with Natural Convection by Temperature Recovery Method

In this section, a numerical scheme is introduced to solve a general two-dimensional solidification problem with natural convection by the temperature recovery method. As mentioned in a previous section, the front tracking method is limited to solidification of pure metals. The temperature recovery method will be a good candidate to resolve this because it can handle the release of latent heat for pure metals as well as alloys. The numerical procedures for this scheme are as follows;

(i) Solve the heat conduction for all domains using the temperature recovery method (time step $\Delta t_1$);

(ii) Determine the phase front position based on the temperature distribution from (i); set up the mesh for the liquid zone; reorder the numbering of nodes to reduce the bandwidth (time step $\Delta t_1$);

(iii) Simultaneously solve the momentum and energy equations (Equations (5-27) and (5-28)) (time step $\Delta t_1$); go to the next time step.

Since the no-slip boundary condition should be applied to the solid/liquid interface, Voller [46] and Gartling [41] used fictitious viscosity in the element near the interface. In this study, a mesh for liquid domain was created for each time step such that the no-slip boundary condition can be applied to the solid/liquid interface. For the thermal boundary condition, a prescribed solidus temperature was applied at the solid/liquid front. It was hoped that with the creation of a new mesh in the liquid domain, the temperature and velocity fields near the phase front can be determined more accurately.
The mesh for liquid zone was created based on the initial mesh layout. Since the phase front was determined by the temperature distribution from procedure (i), the elements with all nodes that are inside the liquid domain can be found. The elements containing the phase interface were divided into two or three new elements such that the domain of liquid can be clearly described. These newly-created elements would be merged with elements whose four nodes fell inside the liquid domain. This operation would cause bad ordering system of the new mesh in a liquid zone. The reordering of the numbering of the mesh was executed by the Cuthill-McKee Algorithm [73]. Since the mesh generation was performed for each time step (Δt), this numbering procedure can dramatically reduce the size of bandwidth and the computation time. As discussed previously, the temperature recovery method requires small time steps to get accurate results. Thus, we can determine the position of phase front by a smaller time step (Δt₁) and use a larger time step (Δt₂) in calculating the velocity to save computation time.

In application, we solved the aluminum solidification in a square enclosure with one cooled wall (see Figure 5.3) with the presence of natural convection. The material properties used in simulation were the same as those in Table 5.1 and 5.2. By solving the same problem with two different methods, we can compare the results of these two methods.

One of the main differences about these two methods is the way to discretize the changing liquid domain. The front tracking method sets up a new mesh for each time step. Since the locations of new mesh are different from the old one, the temperature and velocity of these new locations were interpolated from the temperature and velocity of the old mesh. The proposed temperature recovery method sets up the new mesh only at
locations near the phase front. The locations of the old mesh would not move such that no interpolation was necessary. However, some literature suggested that fine mesh near phase front was necessary for fluid with high Rayleigh number if the fixed domain method was used. Thus, two meshes (A and B), shown in Figure 5.13, were adopted in simulation. Both meshes consisted of 30 elements in the x direction and 19 elements in the y direction. The grid size in x direction was uniform (1/30 of width, W) in mesh A and varied from 1/60 of width near the cold wall to 2/30 width near the opposite side of the cold wall in mesh B.

The velocity vector plot and temperature distribution by using mesh B with Ra=100,000 at 512 seconds after solidification started is shown in Figure 5.14(a) and 5.14(b), respectively. These results can be compared with the results from front tracking method, Figures 5.4(b) and 5.5(b). One can notice that the position of phase front in Figure 5.14(a) approximately coincides with that in Figure 5.4(b). However, phase front in Figure 5.14(a) changes sharply while phase front in Figure 5.4(b) changes smoothly. Although, the temperature and velocity distributions were similar, the magnitude of velocity from the temperature recovery method is smaller than the one from front tracking method. To investigate this discrepancy, the components of velocities in y direction at 0.28 high were plotted in Figure 5.15. The figure includes three curves; two were from the temperature recovery method with meshes A and B and one was from the front tracking method. The results from mesh A underestimated the magnitude of velocity. With a finer mesh in the phase front, the results from mesh B was closer to those of the front tracking method. This underestimation of magnitude of velocity can be explained in two ways as follows;
Figure 5.13. Quasi Uniform (A) and graded (B) mesh layout.
Figure 5.14(a). Velocity field by temperature recovery method for $Ra_T=10^5$ at time = 512 seconds.
Figure 5.14(b). Temperature distribution by temperature recovery method for $Ra_r=10^5$ at time = 512 seconds; temperature interval = 5 °C.
Figure 5.15. Vertical velocity by employing mesh A, mesh B, and front tracking method.
(1) In a fixed domain method, the phase front usually moves grid by grid. The velocity at the grid next to the interface may be sacrificed by this movement.

(2) Since velocity is induced by the density difference near the phase front, high thermal gradients will cause high velocity. In the early stage, the highest velocity occurs near the phase front (see Figure 5.4(a)).

Combining these two effects, some velocities near the interface may be wiped out during the grid-by-grid movement. Although the mesh generation near the interface of present scheme is expected to reduce the velocity loss, the nature of the temperature recovery method will underestimate the velocity component.

In the temperature recovery method, the temperature at certain nodes was kept to some values until the solidification completes. Then, the end of solidification was arrived at when the latent heat was used up. Once the solidification at a certain node was completed, the temperature would drop sharply as observed later in chapter 6. Thus, if we use the temperature distribution to determine the position of phase front, the phase front would still jump from one grid to the next. This can be controlled more carefully by redistributing the amount of heat used in the temperature recovery method to calculate phase front more reasonably.

The example mentioned above is similar to a one-dimensional solidification problem since the solid/liquid interface is not far from a straight line. The main purpose of next example is to verify that the present method can handle a general two dimensional solidification problem including the natural convection effect. The solidification of aluminum in a square
enclosure with four cold walls was studied. The length for each side was 50 cm. The cold wall was set to the prescribed temperature 610 °C. The initial and melting temperatures were 710 °C and 660 °C, respectively. The material properties used in simulations were the same as those in Table 5.1 and 5.2. A 30 x 30 grid was adopted and the time step used was 1.365 seconds for temperature calculation and 6.8267 seconds for velocity calculation. The charged CPU time was about four hours in VAX 8550.

The vector plot and temperature distribution for Ra=100,000 at time=171 and 445 seconds are shown in Figure 5.16 and Figure 5.17, respectively. The temperature distribution without the presence of natural convection at 445 seconds is shown in Figure 5.18. Comparing the temperature distributions in Figures 5.17 and 5.18, following observations can be made;

1) The hottest spot will move upward to the height of about 0.6 y/H because of the natural convection;

2) The geometry of phase front of Figure 5.17 is no longer symmetrical to the line of half height. The liquid zone will become a shape with larger area in the upper half and smaller area in the lower half;

3) The highest temperature with convection effect was about 1.4 °C lower than that without natural convection. The presence of natural convection will reduce the thermal gradient in the liquid zone. This phenomenon has been mentioned in the literature survey [49].

In this section, a scheme based on the temperature recovery method was developed to handle the effect of natural convection in liquid pool and the computed results were compared with those from the front tracking method. The developed scheme provided a reasonable result for two
Figure 5.16. Velocity vector and temperature distribution by temperature recovery method for $Ra=10^5$ at time = 171 seconds (Four cold wall temperatures = 510 °C).
Figure 5.17. Velocity vector and temperature distribution by temperature recovery method for $Ra=10^5$ at time = 445 seconds (Four cold wall temperatures = 510 °C).
Figure 5.18. Temperature distributions without natural convection at time = 445 seconds (Four cold wall temperatures = 510 °C).
dimensional problems when refined mesh was used near the solid/liquid interface. In conclusion, to use the temperature recovery method in solidification with natural convection, appropriate time step and refined mesh must be used at the cost of computation time.
5.4 The Heat, Momentum and Species Transport in a Binary Solidification System

In sections 5.2 and 5.3, the solidification of pure metal with natural convection has been studied. In this section, the technique used in section 5.3 will be extended to solve the solidification system of binary alloys. As explained before, the solidification of alloys is much more complicated than for pure metal because:

(i) Latent heat is not released at a fixed temperature but at a range of temperatures (liquidus to solidus temperatures);

(ii) The solidification will make the composition change such that the temperature, velocity and composition will have coupled effects on each other;

(iii) The presence of mushy zone will change the flow pattern. The interdendritic flow usually was simulated as the flow in the porous media using Darcy's rule [50].

The continuum system discussed in Appendix D is suitable for simulating the solidification of alloys. If we adopt the Boussinesq assumptions (Equation (5-1)) here and combine the results of Appendix D, that is, Equations (D-6,16,17,23,and 28), the governing equations for a binary alloy system can be written as,

continuity

\[ \nabla \cdot \vec{V} = 0 \]  \hspace{1cm} (5-29)

momentum

\[ \frac{\partial}{\partial t} (\rho \vec{u}) + \nabla \cdot (\rho \vec{V} \vec{u}) = \nabla \cdot \left( \sum_k \mu_k \nabla (g_k u_k) \right) - \frac{\mu_1}{K} \rho_i (u - u_i) - \frac{\partial p}{\partial x} \]  \hspace{1cm} (5-30)
\[
\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla \cdot (\rho \nabla \mathbf{v}) = \nabla \cdot \left( \sum_k \mu_k \nabla (g_k \mathbf{v}_k) \right) - \frac{\mu_1}{\rho_1} \nabla (\rho \mathbf{v} - \mathbf{v}_s) - \frac{\partial \rho}{\partial y} + \rho \nabla \left[ \beta_T (T - T_0) + \beta_s (f_i^a - f_{i,s}^a) \right]
\]

(5-31)

energy

\[
\frac{\partial}{\partial t}(\rho cT) + \nabla \cdot (\rho \nabla cT) = \nabla \cdot (k \nabla T)
\]

(5-32)

species

\[
\frac{\partial}{\partial t}(\rho f^a) + \nabla \cdot (\rho \nabla f^a) = \nabla \cdot (\rho D_i^a \nabla f_i^a)
\]

(5-33)

where \( u_s \) and \( v_s \) are the components of velocity at solidus line, \( g_k \) is the volume fraction of phase \( k \), \( \mu_1 \) is the dynamic viscosity for liquid and \( \rho_1 \) is the liquid density. In Equation (5-32), it is reasonable to neglect the relative motion of the mixture velocity and the real velocity since the velocity of the interdendritic flow is relatively small. The initial and boundary conditions for temperature and velocity are the same as those in section 5.2. The initial condition for composition is,

\[
f_i^a = f_{i,s}^a , \text{ at } t = 0
\]

(5-34)

and the boundary conditions are,

\[
(\nabla f_i^a) \cdot \mathbf{n}_2 = 0, \text{ on } \Gamma_2(t)
\]

\[
f_i^a = f_{i,e}^a , \text{ on } \varepsilon(t)
\]

(5-35)

where \( f_{i,s}^a \) is the initial composition of constituent \( \alpha \) in liquid phase, \( f_{i,e}^a \) is the eutectic composition of constituent \( \alpha \) in liquid phase, \( \Gamma_2(t) \) is the boundary for liquid and mushy zone and \( \varepsilon(t) \) is the solidus line.

Using the same non-dimensionalized variables in Equation (5-11) for Equations (5-29) through (5-33), we obtain the non-dimensionalized governing equations as follows;
continuity
\[ \frac{\partial u^*}{\partial x^*} + \frac{\partial v^*}{\partial y^*} = 0 \]  
(5-36)

momentum
\[ \frac{\partial u^*}{\partial t^*} + u^* \frac{\partial u^*}{\partial x^*} + v^* \frac{\partial u^*}{\partial y^*} = - \frac{\partial P_d^*}{\partial x^*} + \text{Pr} \ \nabla^* \cdot (\nabla^* u^*) - \frac{1}{k^*} (u^* - u_1^*) \]  
(5-37)
\[ \frac{\partial v^*}{\partial t^*} + u^* \frac{\partial v^*}{\partial x^*} + v^* \frac{\partial v^*}{\partial y^*} = - \frac{\partial P_d^*}{\partial y^*} + \text{Pr} \ \nabla^* \cdot (\nabla^* v^*) - \frac{1}{K^*} (v^* - v_1^*) - \text{PrRa} \ \varepsilon_2 f_2 \theta_2 + \text{Ra}_c f_2 (f_1^\alpha - f_0^\alpha) \]  
(5-38)

energy in liquid
\[ \frac{\partial \theta_2}{\partial t^*} + u^* \frac{\partial \theta_2}{\partial x^*} + v^* \frac{\partial \theta_2}{\partial y^*} = \nabla^* \cdot (\nabla^* \theta_2) \]  
(5-39)

energy in solid
\[ \frac{\partial \theta_1}{\partial t^*} = R_a \ \nabla^* \cdot (\nabla^* \theta_1) \]  
(5-40)

species in liquid
\[ \frac{\partial (p^* f^\alpha)}{\partial t^*} + u^* \frac{\partial (p^* f^\alpha)}{\partial x^*} + v^* \frac{\partial (p^* f^\alpha)}{\partial y^*} = \nabla^* \cdot (D^* \nabla^* p^* f^\alpha) \]  
(5-41)

Here, \( \tilde{V} = u^* + v^* \) and continuity equation are used in deriving (5-37) and (5-38). The definition for Prandtl number has changed to, \( \text{Pr} = \sum_k g_k \mu_k / \rho_1 \alpha_2 \).

Some new variables \( \rho^*, K^*, D^*, \) and \( \text{Ra}_c \) are defined as follows,
\[ \rho^* = \frac{\rho}{\rho_1}, \quad D^* = \frac{D}{\alpha_2}, \quad K^* = \frac{K}{\text{Pr} \ \frac{\rho}{\rho_1} \ C_L^2}, \quad \text{Ra}_c = g \beta c L \alpha_2^2. \]  
(5-42)

The new unknown variable \( f_1^\alpha \) can be approximated over the domain \( \Omega_2 \) by a combination of interpolation functions,
\[ f_1^\alpha(\tilde{x}, t) = \sum_q F_q(t) N_q(\tilde{x}) \]  
(5-43)

where \( q \) is the nodal point of the element, \( F_q \) are the nodal liquid composition of constituent \( \alpha \) and \( N_q(\tilde{x}) \) are interpolation functions. The finite element formulations for Equations (5-36) through (5-41) will be very similar to those
in section 5.2 except for some additional terms. By applying the similar procedure, we obtain,

\[
\frac{1}{\Delta t} [\bar{M} \bar{M}]^{t+\Delta t} \begin{bmatrix} \bar{U}^{t+\Delta t} - \bar{U}^t \\ \bar{V}^{t+\Delta t} - \bar{V}^t \end{bmatrix} + [\bar{C} \bar{C} + \Pr \bar{K} \bar{K} + \lambda \bar{L} \bar{L} + \frac{1}{\bar{K}} \bar{M} \bar{M}]^{t+\Delta t}
\]

\[
\begin{bmatrix} \bar{U}^{t+\Delta t} \\ \bar{V}^{t+\Delta t} \end{bmatrix} = \begin{bmatrix} \bar{R}_1 \\ \bar{R}_2 \end{bmatrix} + \Pr \bar{R} \bar{M} [t^{-1}\bar{T}_2^{t+\Delta t}]
\]

\[+ \bar{R} \bar{C} \bar{M} (t^{-1}\bar{F}_1^{t+\Delta t} - \bar{F}_1^{t+\Delta t}) + \Pr^{-1} \bar{K}_2 [t^{-1}\bar{T}_2^{t+\Delta t}] + \frac{u_s}{\bar{K}} \]

(5-44)

\[
\frac{1}{\Delta t} \bar{M}_2 \begin{bmatrix} \bar{T}_2^{t+\Delta t} - \bar{T}_2^t \\ \bar{F}_1^{t+\Delta t} + \bar{C}_{11}^{t+\Delta t} + \bar{C}_{22}^{t+\Delta t} \end{bmatrix} + \bar{K}_2 [t^{-1}\bar{T}_2^{t+\Delta t} = Q_2
\]

(5-45)

\[
\frac{1}{\Delta t} \bar{M}_2 \begin{bmatrix} \bar{T}_2^{t+\Delta t} - \bar{F}_1^{t+\Delta t} \\ \bar{F}_1^{t+\Delta t} + \bar{C}_{11}^{t+\Delta t} + \bar{C}_{22}^{t+\Delta t} \end{bmatrix} + \bar{D} \bar{K}_2 [t^{-1}\bar{F}_1^{t+\Delta t} = \bar{F}_Q
\]

(5-46)

where,

\[\bar{F}_Q = \sum_m \int_{\partial \Omega} \left( \frac{\partial f^a_1}{\partial x^m} n^a_2 x + \frac{\partial f^a_1}{\partial y^m} n^a_2 y \right) \bar{N}^a ( \partial \Omega \right) ds \]

where \( n^a_2 x \) and \( n^a_2 y \) are the components of the unit outward vector at the liquid and mushy zone boundary \( \partial \Omega \) in the \( x \) and \( y \) directions, respectively.

The procedure to solve Equations (5-44) through (5-46) is very similar to the one described in section 5.2. First, the velocity in Equation (5-44) was obtained with the values of temperature and composition from the last iteration. Then, the energy and species equations were solved using the velocity at the current time step. The velocity, temperature and species fields would finally be obtained at the current time step when the numerical iteration converged to a given limiting value. Meanwhile, using the
technique described in section 5.3, the location of solidus line would be calculated by the temperature recovery method.

Before proceeding with the numerical study, a brief discussion of permeability in a mushy zone will be presented. Poirier [74] investigated the permeability data for a partially solid Pb-Sn alloy and concluded that when flow is parallel to the primary dendrite arms, the permeability will be a function of $f_l$ and $d_1$, the primary dendrite arm spacings. But when flow is normal to the primary dendrite arms, the permeability is a function of $f_l$, $d_1$ and $d_2$, the secondary dendrite arm spacings. Thus, $K$ is anisotropic for columnar-dendritic structure. However, because of the lack of experimental data, $K$ will be assumed to be isotropic in this study. The permeability, $K$ is usually expressed as a function of volume fraction of liquid, $f_l$. Many equations can be found in the literature. Flemings et al. [75-77] suggested,

$$K = K_o f_l^2.$$  \hspace{1cm} (5-47)

Another popular equation is the Kozeny-Carman (or Blake-Kozeny) equation [78] as follows,

$$K = K_o \left[ \frac{f_l^3}{(1 - f_l^2)} \right].$$  \hspace{1cm} (5-48)

$K_o$ is a constant which depends on the morphology of mushy zone as previously explained. Takahashi et al. [61] found that there is a critical volume fraction of liquid ($f_{lc}$) such that when $f_l$ is less than $f_{lc}$, the permeability is very low. For example, Ohnaka and Matsumoto [79] used the following equation of permeability for the solidification of Al-4.4%Cu alloy,

$$K(m^2) = \begin{cases} 4.0 \times 10^{-10} f_l^3 & \text{for } f_l \leq 0.8258 \\ 4.073 \times 10^{-9} f_l^{1.55} & \text{for } 0.8258 < f_l \leq 1.0. \end{cases}$$  \hspace{1cm} (5-49)
The developed program has been tested by solving the case of a rectangular aluminum casting with the geometry 25 cm in width and 20 cm in height (see Figure 5.19). The wall at x=0 was exposed to the environment and all other walls were insulated. The convective temperature boundary condition, equation (5-50) was applied at x=0.

\[- k \frac{dT}{dx} \mid_{x=0} = h_a (T - T_\infty) \]

where \( h_a = 627.9 \text{ W/(m}^2\text{K)} \) and \( T_\infty = 20^\circ\text{C} \). The initial temperature for casting was 647°C. The liquid diffusivity used in the simulation was \( 1.2 \times 10^{-1} \text{ cm}^2/\text{s} \). The material properties used in the simulation are shown in Table 5.3. The initial temperature for casting was 647°C. The liquid diffusivity used in the simulation was \( 1.2 \times 10^{-1} \text{ cm}^2/\text{s} \). The material properties used in the simulation are shown in Table 5.3. The initial temperatures in the casting, and mold were 647 °C and 20 °C,
Figure 5.19. Dimensions and thermal boundary conditions for the rectangular ingot casting of Al-4.4% Cu alloy.

Table 5.3. Thermal properties of Al-4.4%Cu

<table>
<thead>
<tr>
<th></th>
<th>Solid</th>
<th>Liquid</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>k</td>
<td>0.33</td>
<td>0.299</td>
<td>cal/cms °C</td>
</tr>
<tr>
<td>c</td>
<td>0.259</td>
<td>0.259</td>
<td>cal/g°C</td>
</tr>
<tr>
<td>L</td>
<td>96.81</td>
<td>96.81</td>
<td>cal/g</td>
</tr>
<tr>
<td>ρ</td>
<td>2.70</td>
<td>2.667</td>
<td>g/cm³</td>
</tr>
<tr>
<td>Tm</td>
<td>548</td>
<td>630.7</td>
<td>°C</td>
</tr>
<tr>
<td>α₂</td>
<td>0.4719</td>
<td>0.4327</td>
<td>cm²/s</td>
</tr>
</tbody>
</table>
Figure 5.20. Temperature distribution (rectangular ingot casting of Al-4.4%Cu alloy at 53 seconds; temperature interval = 10°C).
Figure 5.21. Velocity vector (rectangular ingot casting of Al-4.4%Cu alloy at 53 seconds).
Figure 5.22. Composition distribution (rectangular ingot casting of Al-4.4%Cu alloy at 53 seconds; temperature interval = 0.01).
respectively. However, since perfect contact at the mold/casting interface was adopted in the study, the initial temperatures at the mold/casting interface were 647 °C. The thermal properties of steel mold were as follows:

\[ k = 0.070 \text{ cal/cm g °C}, \quad c = 0.12 \text{ cal/g °C} \]
\[ \rho = 7.75 \text{ g/cm}^3. \]

Prandtl number and permeability used in simulation were assumed to be,

\[ Pr = 0.03041 \]
\[ K^* = 0.152 \times f_1^4 \text{ (cm}^2). \]

Since \( K=K_1f_1^n \) \((n=2 \text{ to } 11)\) has been used in literature \([26,61]\), the \( K_1 \) and \( n \) are chosen as 0.05 and 4 in simulation. Meshes of 400 and 500 quadrilateral elements in casting and mold, respectively, were used for the finite element simulations. The time step used was 0.424 seconds.

One of the objectives for this simulation was to study the effects of natural convection, species transport and heat transfer at the mold/casting
interface to the temperature, shrinkage distribution and total solidification time. Thus, simulations were performed for the following five cases; (a) heat conduction and perfect contact condition at the mold/casting interface ($Ra_T=0$, $Ra_C=0$, $h=\infty$), (b) heat conduction, natural convection and perfect contact condition at the mold/casting interface ($Ra_T=500,000$, $Ra_C=0$, $h=\infty$), (c) conduction, natural convection, species transport and prefect contact condition at the mold/casting interface ($Ra_T=500,000$, $Ra_C=150,000$, $h=\infty$), (d) heat conduction and high heat transfer coefficient ($Ra_T=0$, $Ra_C=0$, $h=4.0 \text{cal/cm}^2\text{s}^\circ\text{C}$), and (e) heat conduction and usual heat transfer coefficient ($Ra_T=0$, $Ra_C=0$, $h=0.04 \text{cal/cm}^2\text{s}^\circ\text{C}$). The heat transfer coefficient used in case (e) is in the same order of the practical value found in permanent mold casting [62].

The temperature distributions 16.95 seconds after solidification started are shown in Figure 5.24 for cases (a), (b) and (c). One can find that the hottest spot moves to $y=6.0$ cm and the hottest temperature drops with the presence of natural convection. Accounting for the fact that the copper composition used (4.4%) is less than the alloy eutectic composition (33%) and copper is heavier than aluminum, the presence of species transport will augment the effect of natural convection on solidification. From the observation that the hottest temperatures in Figures 5.24(a)-(c) are 597.5, 594.8, and 594.3 °C for each case, the presence of species transport slightly increases the natural convection effect in the present simulation. The velocity distributions for cases (b) and (c) at 16.95 seconds after solidification started are shown in Figure 5.25 while the shrinkage distributions for cases (a)-(c) are shown in Figure 5.26. By comparing the results for cases (a), (b) and (c) it can be found out that the lowest location of shrinkage moves in the positive y direction in the
Figure 5.24. Temperature distributions (solidification of Al-4.4%Cu alloy at 16.95 seconds; temperature interval = 10 °C; (a) for heat conduction only, (b) for heat conduction and convection, and (c) for conduction, convection and species transport).
Figure 5.25. Velocity vectors (solidification of Al-4.4%Cu alloy at 16.95 seconds; (a) for heat conduction and convection, and (b) for conduction, convection and species transport).
Figure 5.26. Shrinkage distributions ((a) for heat conduction only, (b) for heat conduction and convection, and (c) for conduction, convection and species transport).
order of cases (a), (b) and (c). This is due to the natural convection effect which moves the hotted molten metal upward. Cases (d) and (e) have the same lowest location of shrinkage as case (a) because heat conduction is considered only.

From Table 5.4, the computation times for cases (b) and (c) are required about fifteen to twenty times more than for case (a). The total solidification time for cases (a), (b) and (c) are found to be the same. The total solidification time for case (e) is much longer than that of cases (a), (b), (c) and (d). This is physically reasonable. Thus, it can be concluded that the interface heat transfer condition has a significant effect on the total solidification time. The main reason why the C. P. U. time for case (d) is larger than that for case (e) is that the smaller size of time increment was required for case (e) since the temperature change at the mold/casting interface was very large in this case. From these results, it is found out that the shrinkage prediction can be economically and conservatively made by simulating the solidification with conduction effect only in the casting. The total solidification time and C. P. U. for cases (a) through (e) are compared in Table 5.4.
Table 5.4. Comparison of solidification and C. P. U. times for five different cases of solidification.

<table>
<thead>
<tr>
<th>Conditions</th>
<th>Location of lowest shrinkage y (cm)</th>
<th>Solidification time (seconds)</th>
<th>C. P. U. (minutes in VAX 8550)</th>
</tr>
</thead>
<tbody>
<tr>
<td>heat conduction and perfect contact</td>
<td>5.5</td>
<td>81.79</td>
<td>17.09</td>
</tr>
<tr>
<td>(Ra_1 = 0, Ra_c = 0, h = \infty)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>heat conduction and convection</td>
<td>6.5</td>
<td>81.79</td>
<td>289.4</td>
</tr>
<tr>
<td>(Ra_1 = 500,000, Ra_c = 0, h = \infty)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>heat conduction, convection and species transport</td>
<td>6.5</td>
<td>81.79</td>
<td>324.7</td>
</tr>
<tr>
<td>(Ra_1 = 500,000, Ra_c = 150,000, h = \infty)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>heat conduction and high h</td>
<td>5.5</td>
<td>74.95</td>
<td>57.4</td>
</tr>
<tr>
<td>(Ra_1 = 0, Ra_c = 0, h = 4 cal / cm^2 s °C)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>heat conduction and usual h</td>
<td>5.5</td>
<td>135.4</td>
<td>8.02</td>
</tr>
<tr>
<td>(Ra_1 = 0, Ra_c = 0, h = 0.04 cal / cm^2 s °C)</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
CHAPTER VI
THREE DIMENSIONAL APPLICATIONS
OF SOLIDIFICATION PROBLEMS

The main task included in this chapter was the verification of the developed 3D finite element program for solidification. The finite element formulation of three-dimensional heat conduction problem has been discussed in Section 2.1. Euler backward finite difference scheme was used in the time discretization. Similar to the two-dimensional solidification problems, the temperature recovery method was adopted.

The verification of the present 3D program includes two steps. First, we need to check whether the developed program can solve the heat conduction equations accurately with different types of boundary conditions. Case Five and Case Six are selected to test this for cubic solids with fixed temperature and constant heat transfer boundary conditions, respectively. The calculated temperature distributions are compared with the analytical solutions from the literature [68]. Good agreement was obtained in both cases. This verified the program's capability to solve the three-dimensional transient heat conduction problems. Then, the program was used to solve some solidification problems. In Case Seven, the temperature distribution of a semi-infinite freezing problem was calculated and compared with the analytical solutions available in the literature [68-70]. In Case Eight, the solidification of a corner region was studied. In both cases, comparisons between calculated temperatures and analytical solutions were good if proper
time step was used. From these results, the developed program was proved to have the ability to simulate three-dimensional casting processes with conduction only. The computed temperature history of a semi-infinite solidification problem by different methods is compared in Case Nine. The results show the enthalpy method provides a better predictions under present condition than the temperature recovery and front tracking methods.

6.1 Case Five - Temperature in a Cubic With a Prescribed Temperature Boundary Condition

The first test to verify the developed three-dimensional heat transfer program involved transient conduction heat transfer in a rectangular parallelepiped with a fixed temperature at boundary. The analytical solution is available in [68]. The dimensions are -a<x<a, -b<y<b, and -c<z<c, where a=b=c=1/2 cm, with a unit initial temperature and zero surface temperature. The analytic solution is given by,

\[ T(x, y, z, t) = \frac{64}{\pi^3} \sum_{l=0}^{\infty} \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{(-1)^{l+m+n}}{(2l+1)(2m+1)(2n+1)} \times 
\cos \frac{(2l+1)\pi x}{2a} \cos \frac{(2m+1)\pi y}{2b} \cos \frac{(2n+1)\pi z}{2c} e^{-\beta_{l,m,n} t}, \]

where

\[ \beta_{l,m,n} = \frac{\alpha \pi^2}{4} \left[ \frac{(2l+1)^2}{a^2} + \frac{(2m+1)^2}{b^2} + \frac{(2n+1)^2}{c^2} \right]. \] (6-1)

The thermal properties in this example are: k=0.597 cal/cm sec °C and \( \rho c=0.5418 \) cal/cm\(^3\) °C. Analytic solution can be accurately determined from
Equation (6-1). The rate of convergence of analytic solution is fast except when \( t \) is very small. Usually, 25 steps for \( l, m, \) and \( n \), are sufficient to get results with errors less than \( 10^{-6} \). In F. E. analysis, a 7x7x7 cubic mesh with symmetric boundary conditions at surfaces \( x=0, y=0, \) and \( z=0 \) was used to calculate the temperature distribution. Prescribed temperature, 0 °C was applied at surface \( x=1/2, y=1/2, \) and \( z=1/2 \) cm. The calculated temperatures compared well with the analytical solution at two locations (see Figure 6.1).

6.2 Case Six - Temperature in a Cubic with a Convective Boundary Condition

An example is presented here to show the program's capability to solve 3-D heat conduction equation with a heat flux boundary condition. The convective boundary condition was assumed on all the external surfaces of the cubic in the form of

\[
-k \frac{\partial T}{\partial n^*} = h (T_{\text{wall}} - T_\infty)
\]

where \( T_{\infty} \) and \( T_{\text{wall}} \) are the temperatures of the ambient and the wall, respectively. \( n^* \) is the outward normal vector of the surface and \( h \) is the heat transfer coefficient at the surface. The analytic solution can be found in [68]. The geometry was \(-a<x<a, -b<y<b, \) and \(-c<z<c \) (\( a=b=c=0.5 \) cm) with a unit initial temperature and zero ambient temperature. The analytic solution is given as,

\[
T(x, y, z, t) = \psi(x, t, a, h) \psi(y, t, b, h) \psi(z, t, c, h)
\]

where,
Figure 6.1. Comparison between analytical and F. E. results calculated with $\Delta t=0.001$ sec. for a prescribed temperature boundary condition.
\[ \psi(x, t, a, h) = \sum_{n=1}^{\infty} \frac{2h \cos \beta_n x}{(h^2 + \beta_n^2) \cos \beta_n a} e^{-\beta_n^2 t} \]  
\hspace{1cm} (6-3)

and the \( \beta_n \) are the positive roots of

\[ \beta \tan \beta a = h. \]  
\hspace{1cm} (6-4)

\( h \) is the heat transfer coefficient at the interface.

The analytical solution can be accurately determined by Equation (6-3) with 30 terms in each coordinate. The thermal properties used in the analysis were the same as those in Case Five. The heat transfer coefficient was assumed to be 1.1357 cal/cm\(^2\) sec \( ^\circ \)C. A mesh with 7 elements in each side of the cubic (343 element and 512 nodes in total) was used in F.E. analysis. The comparison between analytical and computational results at two locations is shown in Figure 6.2. From the results shown in sections 6.1 and 6.2, the developed program can reasonably predict temperature of a three-dimensional heat conduction problem with fixed temperature or convective boundary conditions.

6.3 Case Seven - Temperature in a Semi-infinite Plane with Phase Change

The solidification of a semi-infinite slab was studied in this test. The initial temperature, \( T_i \), was -17.78 \( ^\circ \)C and the melting temperature, \( T_m \), was -18.33 \( ^\circ \)C. The boundary temperature, \( T_o \), at the surface of \( x=0 \) was -42.78 \( ^\circ \)C. The configuration of this problem is shown in Figure 6.3. The thermal properties used in this example were: \( k_s = k_l = 197. \) cal/cm sec \( ^\circ \)C, \( \rho c_s = \rho c_l = 28.2 \) cal/cm\(^3\) \( ^\circ \)C and \( \rho L = 1101. \) cal/cm\(^3\) .
Figure 6.2. Comparison between analytical and F. E. results calculated with
$\Delta t=0.001$ sec for a heat flux boundary condition.
Figure 6.3. Configuration and boundary conditions of Case Seven.

Figure 6.4. Analytical and F. E. temperature histories at $x=2.54$ cm of a semi-infinite phase change problem (Case Seven).
The exact solution to this problem is given by [68-70],

\[ T_1(X, t) = T_0 + (T_m - T_0) \left[ \frac{\text{erf}(X/2\sqrt{\alpha_s} t)}{\text{erf}(\beta/2\sqrt{\alpha_s})} \right] \]

for the solid phase, and

\[ T_1(X, t) = T_1 + (T_m - T_1) \left[ \frac{\text{erfc}(X/2\sqrt{\alpha_1} t)}{\text{erfc}(\beta/2\sqrt{\alpha_1})} \right] \]

(6-5)

for the liquid phase. The value of \( \beta \) in the above equations is determined from the following complementary equation:

\[
\frac{L}{2\sqrt{\pi}} \beta = \frac{k_s(T_m - T_0)}{\sqrt{\alpha_s} \text{ erf}(\beta/2\sqrt{\alpha_s})} \exp\left(\frac{-\beta^2}{4\alpha_s}\right) \\
+ \frac{k_1(T_m - T_1)}{\sqrt{\alpha_1} \text{ erfc}(\beta/2\sqrt{\alpha_1})} \exp\left(\frac{-\beta^2}{4\alpha_1}\right) 
\]

(6-6)

which is derived from energy balance equation, Equation (2-5), at the moving interface. The interface position is located at \( \beta \sqrt{t} \). L is the latent heat and \( \alpha_s \), and \( \alpha_1 \) are the diffusivity at solid and liquid, respectively. The analytical solutions can be obtained by solving Equation (6-6).

A mesh with 40, 5, and 2 8-node linear cubic elements was used in the analysis. The analytical temperature distribution at \( x=2.54 \) cm was calculated and compared with the F. E. results calculated with time steps of 0.1 and 0.005 seconds (see Figure 6.4). One can find that the temperature recovery method predicts the temperature well when the time interval is small. The predicted temperature has the tendency to drop to the melting temperature earlier and stay at the melting temperature longer than what it should be. As mentioned in the literature [16, 80], a stepwise behavior in history of the temperature versus time has been found by using the enthalpy method. This stepwise
behavior can also be found in Figure 6.4 with the use of the temperature recovery method. This behavior is probably a characteristic of the fixed-domain methods. Crank [16] also noticed that the stepwise behavior was more obvious in the frozen range than in the unfrozen range. In Figure 6.4, one can hardly find oscillations in temperature calculation in the unfrozen range.

In Figure 6.5, the temperature distributions along the x axis at 1 second are plotted. The results from F. E. analysis with two time steps used, 0.1 and 0.005 seconds were compared against the analytical solution. One can find that a zone (a "plateau") at the melting temperature has been formed by the use of temperature recovery method. The size of this melting temperature zone depends on the time step used in the analysis. Generally speaking, the smaller the time step used is, the smaller the size of this zone. For instance, the zone at melting temperature with $\Delta t=0.1$ sec. starts from node p to node q while for time step of 0.005 sec., that zone starts from node i to node m.

Since pure material was analyzed in this example, there should be only one point which released the latent heat (as analytical solution in Figure 6.5). However, the front node (i) only released the amount of heat required to recover the temperature loss. In the mean time, all other nodes located in the plateau (j,k,m) released heat and accumulated to their own nodes. It is suggested that all the heat released in the nodes other than the front node should be accumulated to the front node. By doing this, the temperature prediction can be improved. However, this modification is much harder to be implemented in general 2D or 3D problems because it is difficult to decide the node where the released heat accumulates. Thus, it is believed that the temperature recovery method is still a useful method to handle the
Figure 6.5. Analytical and F. E. temperatures along the x axis at 1 second of a semi-infinite phase change problem (Case Seven).
solidification problem if the proper time interval is adopted. Another interesting phenomenon in Figure 6.5 is that the temperature distribution in the frozen phase is almost linear. Bell [80] explained the cause of this phenomenon is that the movement of the phase front is so slow that the temperature within the frozen phase is quasi-steady.

6.4 Case Eight - Solidification of a Corner Region

The solidification of a corner region has been studied by using finite element [8,81] and analytical approaches [82,83]. The domain studied was a corner (90 degrees) region with two infinite edges carrying a freezing temperature -1.0 °C. The initial temperature was 0.3 °C and the melting temperature was 0.0 °C. The material was assumed to be a pure material and the thermal properties were; \( k_s = k_l = 1 \text{ kcal/m sec °C}, \rho c_s = \rho c_l = 1 \text{ kcal/m}^3 \text{ °C} \) and \( \rho L = 0.25 \text{ kcal/m}^3 \).

Because of the symmetry of the problem, only half of the domain was discretized by using 400 cubic 8-nodes elements as depicted in Figure 6.6. The boundary conditions for each surface are also shown in Figure 6.6. The position of the phase front along the 45° bisectrix, \( S^* \), was analytically determined [82,83] as,

\[
S^* = \frac{1.299}{\sqrt{4\alpha t}}
\]  

(6-7)

where \( \alpha = \alpha_s = \alpha_l \) was the thermal diffusivity. The value, 1.299 was measured from the figure such that some small errors may appear. Two time intervals, 0.01 sec. and 0.001 sec. were used in the present finite element
Figure 6.6. Mesh and boundary conditions for Case Eight.
analysis. Figure 6.7 gives the results obtained. The results using a smaller

time step (0.001 sec.) agreed well with the analytical solution while the use of

larger time step (0.01 sec.) would underestimate the position of phase front.
The reason for this discrepancy was that the size of artificial "plateau", as

explained in the last test, from time step 0.01 sec. would be much larger than

that from time step 0.001 sec. The temperature history at location x=y=0.5 m is

depicted in Figure 6.8. Since the analytical solution was not calculated here,
temperatures at four different times were obtained from available results [83].

It was found that the smaller time step improved the temperature prediction

as expected.

Abis [84] and Berry et al. [85] have used the finite element method in

the application of three-dimensional solidification processes. The developed

program was used to simulate the solidification of three-dimensional sand

casting with geometry in literature [86]. However, due to the limitations of

computational time, this work discontinued. As mentioned before, the

implicit scheme was used in the three-dimensional analysis of the

solidification problems. The bandwidth for a three-dimensional mesh was so

large that most of the computational time would be spent in solving matrix.

According to the suggestion by Lewis and Roberts [56], a mixed implicit

/explicit scheme would be more appropriate in handling three-dimensional

solidification problems considering the efficiency of computational time.
Figure 6.7. Front position along 45° bisectrix for Case Eight.
Figure 6.8. Temperature history at location $x=y=0.5$ m for Case Eight.
6.5 Case Nine - Comparison of Different Methods

The same semi-infinite solidification problem was studied in this section by four different numerical and time incremental methods. The finite element model, material properties and boundary conditions are shown in Figure 6.9 and Table 6.1. Zero heat flux boundary condition was applied at x=20 m and the temperature at x=0 was prescribed as -50°C. The two-dimensional finite element mesh was employed within the x=0 to x=20 m.

The enthalpy, temperature recovery and front tracking methods were examined by their accuracy and total computing time. Different time stepping methods, such as the explicit method, Euler backward implicit method and implicit method with conjugate gradient algorithm are also adopted in the study. The methods used and the computation time in each run are listed in Table 6.2. The results of first two runs were calculated by Kitamura [5]. The analytical solution was obtained by solving Equations (6-5,6). The temperature distributions along the x axis at 10 seconds for each run are plotted in Figure 6.10. One can find the enthalpy method gives accurate results with Δt= 0.5 sec for C-G implicit method and Δt= 0.1 sec for explicit method. If the time increment is smaller than the critical value (0.125 seconds in this case), the explicit method is more economical in terms of computing time than the implicit method. The results from front tracking method with a time increment of 0.2 sec. are reasonable. Temperature recovery method required even smaller time steps (0.025 sec.) to get comparable results. From this comparison, it can be concluded that the enthalpy method with internally discontinuous elements to trace phase transition zone is more accurate than
the front tracking method and the temperature recovery method for the present problem.

Table 6.1 Material properties, boundary conditions and initial conditions for Case Nine.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho c / k$</td>
<td>0.25 [sec/m$^2$]</td>
</tr>
<tr>
<td>$\rho L / k$</td>
<td>25.0 [sec°C/m$^2$]</td>
</tr>
<tr>
<td>$T_m$ = melting temperature</td>
<td>0.0 [°C]</td>
</tr>
<tr>
<td>$T_i$ = initial temperature</td>
<td>10.0 [°C]</td>
</tr>
<tr>
<td>$T</td>
<td>_{x=0}$ = boundary temperature at (x=0)</td>
</tr>
<tr>
<td>$\frac{dT}{dx}</td>
<td>_{x=\infty}$ = boundary heat flux at infinite</td>
</tr>
</tbody>
</table>

Figure 6.9. Finite element model for Case Nine.
Table 6.2. Computer Runs in Case Nine.

<table>
<thead>
<tr>
<th>Run</th>
<th>Latent heat Method</th>
<th>Timestepping Method</th>
<th>Δt [sec]</th>
<th>mesh</th>
<th>C.P.U. [sec]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Enthalpy</td>
<td>Explicit</td>
<td>0.1</td>
<td>20x1</td>
<td>7.88</td>
</tr>
<tr>
<td>2</td>
<td>Enthalpy</td>
<td>C-G Implicit</td>
<td>0.5</td>
<td>20x1</td>
<td>13.67</td>
</tr>
<tr>
<td>3</td>
<td>Front Tracking</td>
<td>Euler Implicit</td>
<td>0.2</td>
<td>20x5</td>
<td>18.23</td>
</tr>
<tr>
<td>4</td>
<td>Temperature Recovery</td>
<td>Euler Implicit</td>
<td>0.025</td>
<td>20x1</td>
<td>23.49</td>
</tr>
</tbody>
</table>

* All C.P.U. time in VAX 8550
Figure 6.10. Temperature distribution along x axis of Case Nine.
CHAPTER VII
CONCLUSIONS

7.1 Concluding Remarks

The main objective of this research was to develop a finite element formulation, solution and computer code to analyze the solidification system of pure metals and binary alloys with the effects of natural convection, interdendritic flow and species transport. The first step of this work was to develop a 2-D finite element program which is capable of predicting the temperature profile during solidification without the consideration of natural convection. The temperature recovery method was used to handle the release of latent heat because of its applicability with a reasonable accuracy. A contact thermal resistance was introduced for handling the interface heat transfer between molds and casting with exothermic powders, chills and pads. The technique introduced by Imafuku et al. and Niyama et al. was used in predicting shrinkage and porosity. The developed program was applied to the simulation of two-dimensional and axisymmetric solidification processes to predict temperature, shrinkage and porosity distributions. The simulation results in sand casting as well as in low pressure die casting show fairly good agreement with experimental results, in terms of temperature distribution, shrinkage and porosity defects. This simulation capability will be a useful tool for casting engineers to reduce the casting tryout. Meanwhile, the developed finite element program was also used to calculate the heat transfer coefficient by minimizing the errors between the calculated and measured temperatures.
This capability shows that the proposed scheme will be a useful tool in computing the heat transfer coefficients as a function of location and time.

When studying the solidification with the natural convection effect, the front tracking method was adopted to simulate the solidifying system of gallium. The flow analysis was calculated by using the penalty method. The computed temperature distribution was compared with the available experimental data. The good agreement from the comparison verified the present mathematical model. However, since the upwind technique was not used in the flow analysis, the program encountered numerical instability problem when the convection flow became dominant. The front tracking method has limited application because of its numerical difficulty in tracing the changing liquid domain and the solidification of alloys. The developed technique based on the temperature recovery method was introduced to remove the limitations of the front tracking method. The remeshing for the liquid domain was generated for each time step such that the no-slip boundary condition can be applied on the solid/liquid interface. The simulation results of a solidifying system in a square cavity showed the two-dimensional capability of the present technique. Since the determination of the location of phase front was performed based on the temperature distribution, the disadvantages of the fixed domain method were retained. The comparison between the computed velocity and temperature from the temperature recovery method and front tracking method showed fair agreement. The results suggested that a refined mesh was required in the interfacial area when using the temperature recovery method.

The model based on the temperature recovery method was further extended to handling the solidification of a binary alloy. The developed
model should include the effects of interdendritic flow, species transport as well as natural convection because of the presence of long range mushy zone. A numerical example was studied to show the coupling effect between the heat, species and momentum transport.

The temperature recovery method was also applied to the simulation of three-dimensional solidification problems. The numerical examples were applied to problems with simple geometries such that the computed results could be compared with analytical solutions. The results from the temperature recovery method depended strongly on the size of the time step used in simulation. Accurate results were obtained when appropriately small time steps were used in the analysis.

7.2 Future Research Recommendations

Several future research topics are suggested to improve the efficiency of the numerical method and to solve more complicated engineering problems.

The present study did not analyze the heat loss and flow pattern during the filling stage which are important in die casting and investment casting. The temperature distribution at the end of the filling stage will be used as the initial temperature distribution in the solidification study. To perform the flow analysis in the filling stage, the free surface flow must be analyzed. Another difficulty in analyzing the flow pattern during the filling stage is that the assumption of laminar flow may not be appropriate. Obviously, a turbulent model for fluid flow will make the analysis more complicated.

Another crucial topic is the prediction of heat transfer coefficients. The heat transfer coefficients were input data for the solidification analysis. It is
well known that the heat transfer coefficients are a function of time, location, interfacial conditions and casting dimensions. In die casting, the heat transfer coefficients will also be a function of molten metal pressure. Some work has been done in relating the change of heat transfer coefficients to the formation of gaps at the casting/mold interface. More investigations need to be carried out in determining the heat transfer coefficients properly.

The implicit scheme was adopted for time discretization in the three-dimensional solidification studies. This may not be a good choice since the bandwidth from a three-dimensional mesh will be very large. Thus, much computational time will be spent in solving the matrix. Under this circumstance, a mixed implicit/explicit scheme may be more efficient in the simulation of solidification for a three-dimensional object.

For predicting porosity distribution in terms of $G / \sqrt{R}$ a limiting value for each type of alloy is required. The available information for this material-dependent value is limited to low carbon steel. The limiting values of $G / \sqrt{R}$ for different types of commercially important alloys need to be determined by experiment so that the porosity prediction can be performed in more practical applications.

Finally, a stability problem was evidenced in the flow analysis of molten metal. Recently, the streamline-upwind/Petrov-Galerkin (SUPG) method has become very popular to solve the Navier-Stokes equations because of its success in handling the stability problem. The use of a penalty method in fluid flow analysis will result in greater instability during simulation of the filling stage because the advective term becomes more important. Thus, it is suggested that the SUPG method would be a better choice in flow analysis of the filling stage.
REFERENCES


APPENDIX A

EIGHT-NODE THREE-DIMENSIONAL ELEMENT

In this section, the interpolation functions and Jacobian matrix of an eight-node linear element will be introduced. The interpolation functions of an 8-node linear element can be expressed as follows,

\[
N_1 = \frac{1}{8} (1 - \xi)(1 - \eta)(1 + \zeta) \quad ; \quad N_2 = \frac{1}{8} (1 + \xi)(1 - \eta)(1 + \zeta)
\]
\[
N_3 = \frac{1}{8} (1 + \xi)(1 + \eta)(1 + \zeta) \quad ; \quad N_4 = \frac{1}{8} (1 - \xi)(1 + \eta)(1 + \zeta)
\]
\[
N_5 = \frac{1}{8} (1 - \xi)(1 - \eta)(1 - \zeta) \quad ; \quad N_6 = \frac{1}{8} (1 + \xi)(1 - \eta)(1 - \zeta)
\]
\[
N_7 = \frac{1}{8} (1 + \xi)(1 + \eta)(1 - \zeta) \quad ; \quad N_8 = \frac{1}{8} (1 - \xi)(1 + \eta)(1 - \zeta)
\]

(A-1)

The positions of nodes, 1-8 and the associated coordinates are shown in Figure A.1. Consider the transformation between the global co-ordinates \(x, y, z\) and local co-ordinates \(\xi, \eta, \zeta\). The global derivatives can be formulated as,

\[
\begin{bmatrix}
\frac{\partial N_1}{\partial x} \\
\frac{\partial N_1}{\partial y} \\
\frac{\partial N_1}{\partial z}
\end{bmatrix} = J^{-1}
\begin{bmatrix}
\frac{\partial N_1}{\partial \xi} \\
\frac{\partial N_1}{\partial \eta} \\
\frac{\partial N_1}{\partial \zeta}
\end{bmatrix}
\]

(A-2)

where \(J^{-1}\) represents the inverse of the Jacobian matrix. The Jacobian matrix can be found explicitly in terms of local co-ordinates as follows,
From this form, the Jacobian matrix can be determined for each element. Then, the global derivative can be calculated and the local stiffness matrix can be evaluated at the element level. The derivatives of these interpolation functions with respect to $\xi$, $\eta$, $\zeta$ coordinates can be found as follows:

\[
\begin{align*}
N_{1,\xi} &= -\frac{1}{8}(1-\eta)(1+\zeta) ; \\
N_{2,\xi} &= \frac{1}{8}(1-\eta)(1+\zeta) \\
N_{3,\xi} &= \frac{1}{8}(1+\eta)(1+\zeta) ; \\
N_{4,\xi} &= -\frac{1}{8}(1+\eta)(1+\zeta) \\
N_{5,\xi} &= -\frac{1}{8}(1-\eta)(1-\zeta) ; \\
N_{6,\xi} &= \frac{1}{8}(1-\eta)(1-\zeta) \\
N_{7,\xi} &= \frac{1}{8}(1+\eta)(1-\zeta) ; \\
N_{8,\xi} &= -\frac{1}{8}(1+\eta)(1-\zeta) \\
N_{1,\eta} &= -\frac{1}{8}(1-\xi)(1+\zeta) ; \\
N_{2,\eta} &= -\frac{1}{8}(1+\xi)(1+\zeta) \\
N_{3,\eta} &= \frac{1}{8}(1+\xi)(1+\zeta) ; \\
N_{4,\eta} &= \frac{1}{8}(1-\xi)(1+\zeta) \\
N_{5,\eta} &= -\frac{1}{8}(1-\xi)(1-\zeta) ; \\
N_{6,\eta} &= -\frac{1}{8}(1+\xi)(1-\zeta) \\
N_{7,\eta} &= \frac{1}{8}(1+\xi)(1-\zeta) ; \\
N_{8,\eta} &= -\frac{1}{8}(1+\xi)(1-\zeta) \\
N_{1,\zeta} &= \frac{1}{8}(1-\xi)(1-\eta) ; \\
N_{2,\zeta} &= \frac{1}{8}(1+\xi)(1-\eta) \\
N_{3,\zeta} &= \frac{1}{8}(1+\xi)(1+\eta) ; \\
N_{4,\zeta} &= \frac{1}{8}(1-\xi)(1+\eta) \\
N_{5,\zeta} &= -\frac{1}{8}(1-\xi)(1-\eta) ; \\
N_{6,\zeta} &= -\frac{1}{8}(1+\xi)(1-\eta) \\
N_{7,\zeta} &= -\frac{1}{8}(1+\xi)(1+\eta) ; \\
N_{8,\zeta} &= -\frac{1}{8}(1-\xi)(1+\eta)
\end{align*}
\]
In order to solve problems with a specified heat flux at a boundary, surface integration needs to be carried out. The location and nodes of the six surfaces of this 8-node linear element are depicted in Table A.1. For each surface, following node number will be saved in a counterclockwise order.

Numerical integration over a line domain from \( a^* \) to \( b^* \) can be obtained by using the one-dimensional Gauss quadrature formulas [54],

\[
\int_{a^*}^{b^*} F(x) \, dx = \sum_{i=1}^{N} w_i F(\xi_i) \tag{A-5}
\]

where \( w_i \) are the weighted factors, \( \xi_i \) are the base points and \( N \) is the number of points used in the integration. The values of weights and locations of Gauss points can be found in the literature [54]. The formulas to make numerical integration over a surface \( \partial \Omega \) and volume \( \Omega \) are similar to line integration but extend to two and three dimension. They are shown in Equations (A-6) and (A-7), respectively;

\[
\int_{\partial \Omega} F(\xi, \eta) \, d\xi \, d\eta = \sum_{i=1}^{N} \sum_{j=1}^{M} F(\xi_i, \eta_j) \, w_i \, w_j \tag{A-6}
\]

\[
\int_{\Omega} F(\xi, \eta, \zeta) \, d\xi \, d\eta \, d\zeta = \sum_{i=1}^{N} \sum_{j=1}^{M} \sum_{k=1}^{L} F(\xi_i, \eta_j, \zeta_k) \, w_i \, w_j \, w_k \tag{A-7}
\]

where \( \xi_i, \eta_j, \) and \( \zeta_k \) are the base points in the directions of \( \xi, \eta, \) and \( \zeta, \)
\( w_i, w_j, \) and \( w_k \) are the weighted factors in the directions of \( \xi, \eta, \) and \( \zeta. \)
\( N, M, \) and \( K \) are the number of points used in the integration for the directions of \( \xi, \eta, \) and \( \zeta. \)
8 nodes element

Figure A.1. The positions of nodal point for 8-node linear element.

Table A.1. The location and node number for each surface at 8-node element.

<table>
<thead>
<tr>
<th>Surface number</th>
<th>location</th>
<th>node A</th>
<th>node B</th>
<th>node C</th>
<th>node D</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\zeta = 1$</td>
<td>3</td>
<td>4</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>$\zeta = 1$</td>
<td>3</td>
<td>2</td>
<td>6</td>
<td>7</td>
</tr>
<tr>
<td>3</td>
<td>$\zeta = -1$</td>
<td>7</td>
<td>8</td>
<td>5</td>
<td>6</td>
</tr>
<tr>
<td>4</td>
<td>$\zeta = -1$</td>
<td>4</td>
<td>1</td>
<td>5</td>
<td>8</td>
</tr>
<tr>
<td>5</td>
<td>$\eta = -1$</td>
<td>2</td>
<td>6</td>
<td>5</td>
<td>1</td>
</tr>
<tr>
<td>6</td>
<td>$\eta = 1$</td>
<td>3</td>
<td>7</td>
<td>8</td>
<td>4</td>
</tr>
</tbody>
</table>
APPENDIX B
CALCULATION OF TOTAL SHRINKAGE CAVITY

In this appendix, the derivation of Equation (3-4) will be given. Any element in the casting is assumed to consist of four parts: solid, liquid, solid-liquid, and/or cavity. We may define the elemental liquid and solid volume ratio per unit volume as follows,

\[ v_l^* = \frac{1}{V}(v_l + v_{sl} f_s), \]  \hspace{1cm} (B-1)

\[ v_s^* = \frac{1}{V}(v_s + v_{sl} f_s). \] \hspace{1cm} (B-2)

Here,

- \( v \) = the elemental volume,
- \( v_l \) = the elemental liquid volume,
- \( v_s \) = the elemental solid volume,
- \( v_{sl} \) = the elemental solid-liquid volume,
- \( f_s \) = the elemental solid fraction ratio at solid-liquid part,
- \( f_l \) = the elemental liquid fraction ratio at solid-liquid part,
- \( v_l^* \) = the elemental solid volume ratio per unit volume,
- \( v_l^* \) = the elemental liquid volume ratio per unit volume.

Thus, the elemental solid fraction ratio per unit volume, \( f_s \), can be expressed as

\[ f_s = \frac{v_s + f_s v_{sl}}{V(1 - v_l^*)}, \] \hspace{1cm} (B-3)

where \( v_l^* \) represents the elemental shrinkage volume ratio per unit volume.
By assuming that the major source of shrinkage is caused by phase change, we can derive

$$\frac{\partial v^*_v}{\partial t} = -\beta \frac{\partial v^*_i}{\partial t}, \quad (B-4)$$

where $\beta$ is the volume shrinkage ratio due to solidification.

Then, the total volume of the shrinkage cavity $V_v$ can be obtained by integrating $v_v^*$ for all the nonsolid domains. Since the nonsolid region moves during solidification, the effect of the moving boundary should be considered. However, the velocity of the phase front in the sand casting is very small so that the change of $V_v$ from the moving boundary can be neglected. Thus, the increasing rate of $V_v$ can be expressed as

$$\Delta V_v = \int_{v_{i-\Delta t}}^{v_i} \left( -\beta \frac{\partial v^*_i}{\partial t} \right) dt dV. \quad (B-5)$$

From mass conservation, it follows that

$$\rho_I v^*_i + \rho_s v^*_s = C^*, \quad (B-6)$$

where $C^*$ is a constant. From Equations (B-3) and (B-6), one can determine

$$-\frac{\partial v^*_i}{\partial t} = \frac{\rho_s}{\rho_I} \frac{\partial v^*_i}{\partial t} = \frac{\rho_s}{\rho_I} f_s(t - v_t). \quad (B-7)$$

Substituting Equation (B-7) into (B-5) and expressing $\Delta V_v$ as the change of $V_v$ during the time interval $t-\Delta t$ to $t$, one can derive Equation (3-4).
APPENDIX C

RELATIONSHIP BETWEEN G/√R AND PRESSURE DROP

In this appendix, a simple model of shrinkage formation is explained. The model gives the conclusion that the pressure drop at the root of dendrite is the order of G/√R. The coordinate system is shown in Figure C.1. x is the distance from the root of the dendrite, V_o is the velocity of the contour of solidus (solidification velocity) and V_s is the flow velocity relative to the solidus line. This model is based on the following assumptions,

1. solidification is steady,
2. the elemental liquid fraction ratio f_1 is proportional to the distance x from the root of the dendrite,
3. Darcy's law is applied to interdendritic flow,
4. permeability of the dendritic structure is proportional to f_1,
5. pressure at a point x_c of interdendritic channel is atmospheric pressure P_o and pressure decreases towards the root of dendrite.

According to assumption (3), the pressure drop of Darcy's flow [75] can be expressed as,

\[ \frac{dP}{dx} = -\frac{\mu f_1}{K} V_s \]  \hspace{1cm} (C-1)

where \( \mu \) is the viscosity and K is permeability of interdendritic flow. Pressure drop from P_o to the value for the root of dendrite is,
\[ \Delta P = \int_0^{x_s} dP = -\int_0^{x_s} \frac{\mu f_1}{K} V_s \, dx \]  

(C-2)

From assumption (1), the flow velocity \( V_s \) in the channel is constant and is related to the solidification velocity \( V_o \) as follow,

\[ V_s = \mu \beta' V_o \]  

(C-3)

Here, \( \beta' = \beta / (1 - \beta) \) and \( \beta \) is the contraction due to solidification at solidifying temperature. Substituting assumption (4), that is \( K = c* f_1 \) where \( c* \) is a constant, and \( V_s \) in Equation (C-3) into Equation (C-2), one can find,

\[ \Delta P = -\frac{\mu \beta' V_o}{c*} \int_0^{x_c} dx = -\frac{\mu \beta' V_o x_c}{c*} \]  

(C-4)

The thermal gradient \( G \) can be expressed as, \( G = (T_c - T_s) / x_c \). Then, Equation (C-4) becomes,

\[ \Delta P = \frac{\mu \beta' (T_s - T_c)}{c*} \cdot \frac{V_o}{G} \]  

(C-5)

The cooling rate, \( R \), can be denoted as, \( R = GV_o \). Thus,

\[ \Delta P = \frac{\mu \beta' (T_s - T_c)}{c*} \cdot \frac{R}{G^2} = M* \left( \frac{G}{\sqrt{R}} \right)^{-2} \]  

(C-6)

where \( M* \) is a constant depending on material type.

Assumptions (4) is not realistic since some results [26,61] showed \( K = K_1 f_1^n \) (n=2 to 11). However, even when we apply the more realistic relation into our derivation, only the material constant \( M* \) will change and Equation (C-6) will still hold.
If we assume the pressure drop in the mushy zone is the dominating factor for the formation of porosity, Equation (C-6) may give us a criterion to predict the formation of porosity. In order to use Equation (C-6) the threshold of pressure drop in forming porosity and the material constant $M^*$ should be determined by experiments.

\[
\begin{align*}
P &= P_0 - \Delta P \\
T &= T_s \\
L &= 0 \\
\text{Solid} & \quad \text{Solid+Liquid} \\
\text{Liquid} \\
\end{align*}
\]

Figure C.1 Model for porosity formation.
A continuum model introduced by Bennon and Incropera [50] will be discussed here. The objective of this analysis is to solve the solidification with the effects of natural convection, interdendritic flow and species transport of binary alloy system. The formulation of this model is developed by applying the volume averaging techniques based on classical mixture theory. The law of conservation of mass, momentum, energy and species will be used in obtaining governing equations for the present problem.

The assumptions from classical mixture theory include [87-89];

(i) Each phase of the mixture can be treated as a single material except when it exchanges momentum and energy with each other;

(ii) The equations of motion for a mixture can be expressed as the sum of the equations of motion for all individual phases.

Considering a system of $\alpha$ species and $k$ separable phases, the mean velocity of phase $k$ comprised of all species with phase $k$, is denoted as $\bar{v}^k$. The absolute velocity relative to a fixed coordinate of each species $\alpha$ in phase $k$ is denoted as $\bar{v}_a^k$. $\rho_k$ and $g_k$ are defined as the actual density and volume fraction of phase $k$, respectively. $\phi_k$ is defined as a scalar quantity in $k$ phase of a multiphase mixture. According to assumption (ii), the Reynolds transport theorem [90] for a multiphase mixture can be expressed as,
where \( \vec{n} \) is the normal vector at the surface, \( \vec{J}_k \) is the surface flux vector, \( S_k \) is a source term of \( \phi_k \) per unit volume and \( dA_k \) is the differential surface area of phase \( k \). \( dA_k \) is assumed to be \( g_k dA \). Since \( g_k \) is assumed to be continuous, Equation (D-1) can be transformed to a local formulation as,

\[
\frac{\partial}{\partial t} \int [\rho_k \phi_k] dV_k + \int [\rho_k \vec{V}_k \phi_k] \cdot \vec{n}_k \, dA_k = \int -\vec{J}_k \cdot \vec{n}_k \, dA_k + \int S_k \, dV_k
\]

(D-1)

Here, \( \rho_k = \rho g_k \) and represents the partial density of phase \( k \).

D.1 Conservation of Mass

By using the results of Equation (D-2) with \( \phi_k = 1 \), \( \vec{J}_k = 0 \), and \( S_k = \dot{M}_k \), one can get the conservation of mass for phase \( k \) as,

\[
\frac{\partial}{\partial t} (\bar{\rho}_k) + \nabla \cdot (\bar{\rho}_k \vec{V}_k) = g_k \dot{M}_k
\]

(D-3)

The continuum equation for mass conservation can be obtained by summing Equation (D-3) for all phases. The change of \( \dot{M}_k \) results from mass exchange with other phases. Thus, the total summation of mass exchange for all phases in the right hand side of Equation (D-3) will be zero. Introducing the mixture density and mass averaged velocity as,

\[
\rho = \sum_k \bar{\rho}_k \quad \text{(D-4)}
\]

\[
\vec{V} = \frac{1}{\rho} \sum_k \bar{\rho}_k \vec{V}_k = \sum_k f_k \vec{V}_k \quad \text{(D-5)}
\]

where \( f_k \) is the mass fraction of phase \( k \), we can get the continuum equation of mass conservation as,

\[
\frac{\partial}{\partial t} (\rho) + \nabla \cdot (\rho \vec{V}) = 0
\]

(D-6)
D.2 Conservation of Linear Momentum

The conservation of linear momentum for phase \( k \) in the \( x \)-direction of the Cartesian coordinates can be obtained by applying \( \phi_k = u_k \), \( f_k = -\sigma_{kx} \), and \( S_k = \rho_k B_{kx} + \dot{G}_{kx} \), to Equation (D-2),

\[
\frac{\partial}{\partial t}(\rho_k u_k) + \nabla \cdot (\rho_k \bar{V}_k u_k) = \nabla \cdot (\sigma_{kx}) + \rho_k B_{kx} + g_k \dot{G}_{kx} \tag{D-7}
\]

where in the \( x \) direction, \( u_k \) is the velocity component, \( B_{kx} \) is the body force and \( \dot{G}_{kx} \) is the momentum production due to phase interactions such as drag and lift. The flux vector \( \sigma_{kx} \) represents the component of the general material stress tensor in \( x \)-direction momentum. Summing Equation (D-7) for all the phases, the continuum equation for the conservation of linear momentum in \( x \)-direction will be,

\[
\frac{\partial}{\partial t}(\sum_k \rho_k u_k) + \nabla \cdot (\sum k \rho_k \bar{V}_k u_k) = \nabla \cdot (\sum_k g_k r_{kx}) + \frac{\partial}{\partial x}(\sum_k g_k p_k) + \sum_k \rho_k B_{kx} + F_x \tag{D-8}
\]

where the flux vector has been decomposed into the hydrostatic and deviatoric stress, \( \sigma_{kx} = -p_k I + \tau_{kx} \) and \( F_x \) is the net force due to phase interaction in the form of, \( F_x = \sum_k g_k \dot{G}_{kx} \).

The advective momentum (second term in the L.H.S. of Equation (D-8)) can be decomposed into components resulting from mean mixture motion and relative phase motion,

\[
\sum_k \rho_k \bar{V}_k u_k = \rho \bar{V} u + \sum_k \rho_k (\bar{V}_k - \bar{V})(u_k - u) \tag{D-9}
\]

where \( u \) is the mass averaged velocity of the mixture in the \( x \) direction as follows,
and the $x$-component mixture body force can be defined as follows,

$$ B_x = \frac{1}{\rho} \sum_k \bar{\rho}_k B_{kx} = \sum_k f_k B_{kx} $$

then, Equation (D-8) can be expressed as,

$$ \frac{\partial}{\partial t} \left( \sum_k \bar{\rho}_k u_k \right) + \nabla \cdot (\rho \bar{V} u) = \nabla \cdot \left( \sum_k g_k \tau_{kx} \right) + $$

$$ - \nabla \cdot \left( \sum_k \bar{\rho}_k (\bar{V}_k - \bar{V})(u_k - u) \right) - \frac{\partial}{\partial x} (\sum_k g_k p_k) + \rho B_x + F_x \tag{D-12} $$

If we apply the Newtonian constitutive equations for each phase in Equation (D-12), we can get the following equation,

$$ \frac{\partial}{\partial t} (\rho u) + \nabla \cdot (\rho \bar{V} u) = \nabla \cdot \left( \sum_k \mu_k \nabla (g_k u_k) \right) + $$

$$ - \nabla \cdot \left( \sum_k \bar{\rho}_k (\bar{V}_k - \bar{V})(u_k - u) \right) - \frac{\partial p}{\partial x} + \rho B_x + F_x \tag{D-13} $$

where $\mu_k$ is the viscosity of phase $k$, $u$ is the mass averaged $x$-component of the mixture velocity and $p$ is the mass averaged dynamic pressure. $p$ can be expressed as follows;

$$ p = \sum_k [g_k p_k - \frac{1}{3} \mu_k \nabla \cdot (g_k \bar{V}_k)] \tag{D-14} $$

Then, we assume the internal force in the solid state is negligible and the main phase interaction force can be described with Darcy's law in terms of the $x$-component relative phase velocity, $u_i = u_i - u_s$

$$ F_x = - \frac{\mu_1}{K} g_i (u_i - u_s) \tag{D-15} $$

$K$ is the permeability in the interdendritic flow. Furthermore, the second term in the R.H.S. of Equation (D-13) can be neglected if we assume the velocity of the solidification front is small compared to other velocity terms. This is a reasonable assumption for most cases of sand casting. Combining
Equation (D-15) and (D-13), we can get the continuum expression for momentum conservation in Equation (D-16) as follows,
\[
\frac{\partial}{\partial t}(\rho u) + \nabla \cdot (\rho \nabla u) = \nabla \cdot \left( \sum_k \mu_k \nabla (g_k u_k) \right) - \frac{\mu_i}{K} \frac{\rho}{\rho_i} (u - u_i) - \frac{\partial p}{\partial x} + \rho B_x \tag{D-16}
\]
In order to derive this, the identities \(g_1 = (\rho / \rho_i) f_1\) and \(f_i u_i = u - u_s\) have been used.

Similar results can be obtained for conservation of momentum in \(y\) coordinate as shown in Equation (D-17).
\[
\frac{\partial}{\partial t}(\rho v) + \nabla \cdot (\rho \nabla v) = \nabla \cdot \left( \sum_k \mu_k \nabla (g_k v_k) \right) - \frac{\mu_i}{K} \frac{\rho}{\rho_i} (v - v_i) + \rho B_y \tag{D-17}
\]

D.3 Conservation of Energy

Substituting the following variables, \(\phi_k = c_{kT_k}, \ j_{k} = -k_c \nabla T, \) and \(S_k = \dot{E}_k\) into Equation (D-2), one can get the conservation of energy for phase \(k\) as,
\[
\frac{\partial}{\partial t}(\bar{\rho}_k c_{kT_k}) + \nabla \cdot (\bar{\rho}_k \nabla c_{kT_k}) = \nabla \cdot (g_k k_c \nabla T) + g_k \dot{E}_k \tag{D-18}
\]
where \(\dot{E}_k\) is the energy production associated with phase \(k\). By adding the energy conservation equations for all phases and recognizing that \(\sum_k g_k \dot{E}_k = 0\), we obtain
\[
\frac{\partial}{\partial t}(\rho cT) + \nabla \cdot \left( \sum_k \bar{\rho}_k \nabla c_{kT_k} \right) = \nabla \cdot (k \nabla T) \tag{D-19}
\]
where \(c_T\) and \(k\) are the mixture enthalpy and conductivity defined as,
\[
k = \sum_k g_k k_c \tag{D-20}
\]
\[
c_T = \frac{1}{\rho} \sum_k \bar{\rho}_k c_{kT_k} = \sum_k f_k c_{kT_k} \tag{D-21}
\]

As in the last section, the advective term can be decomposed into the mixture motion and the relative phase motion. That is,
\[
\sum_k \bar{\rho}_k \nabla c_{kT_k} = \rho \nabla c_T + \sum_k \bar{\rho}_k (\nabla \bar{c}_k - \nabla) (c_{kT_k} - c_T) \tag{D-22}
\]
Then, the energy conservation equation can be expressed as,

\[
\frac{\partial}{\partial t}(\rho cT) + \nabla \cdot (\rho \nabla cT) = \nabla \cdot (k \nabla T) - \nabla \left( \sum_k \bar{p}_k (\bar{V}_k - \bar{V}) (c_k T_k - cT) \right)
\]  

(D-23)

D.4 Conservation of Species

The derivation of the continuum equation for conservation of species is similar to that in section D.3. Substituting the following variables, \( \phi_k = f_k^a \), \( \bar{f}_k = -\rho_k D_k \nabla f_k^a \), and \( S_k = \dot{M}_k^a \), into Equation (D-2), one can get the conservation of species \( \alpha \) for phase \( k \) as,

\[
\frac{\partial}{\partial t}(p f_k^a) + \nabla \cdot (\bar{p}_k \bar{V}_k f_k^a) = \nabla \cdot (\rho f_k D_k \nabla f_k^a) + g_k \dot{M}_k^a
\]  

(D-24)

where \( \dot{M}_k^a \) is the generation or loss of species \( \alpha \) for phase \( k \). By adding the equations of conservation for species \( \alpha \) for all phases we can obtain

\[
\frac{\partial}{\partial t}(\rho f^a) + \nabla \cdot \left( \sum_k (\bar{p}_k \bar{V}_k f_k^a) \right) = \nabla \cdot \left( \sum_k \rho f_k D_k \nabla f_k^a \right)
\]  

(D-25)

where \( f^a \) is the mixture concentration of species \( \alpha \), defined by,

\[
f^a = \frac{1}{\rho} \sum_k \bar{p}_k f_k^a = \sum_k f_k f_k^a
\]  

(D-26)

The last term of equation (D-25) will vanish in view of the conservation of mass for species \( \alpha \) for all phases. Since we are dealing with a two-phase solidification system, the diffusivity in the solid phase is much smaller than that in the liquid phase ( \( D_s^a << D_1^a \) ). Thus, we can neglect the diffusion in the solid phase. The first term in the R. H. S. of equation (D-26) will become \( \rho f_1 D_1^a \nabla f_1^a \). As in the last section, the advective term can be decomposed into the mixture motion and the relative phase motion. That is,
\[ \sum_k \beta_k \nabla f_k^\alpha = \rho \nabla f^\alpha + \sum_k \beta_k (\nabla_k - \nabla) (f_k^\alpha - f^\alpha) \]  
(D-27)

If we neglect the term for relative phase motion, the conservation equation for species \( \alpha \) can be expressed as,

\[ \frac{\partial}{\partial t} (\rho f^\alpha) + \nabla \cdot (\rho \nabla f^\alpha) = \nabla \cdot (\rho f_1 D_q \nabla f_1^\alpha). \]  
(D-28)