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THERMAL-MECHANICAL MODEL OF SOLIDIFYING STEEL SHELL BEHAVIOR AND ITS APPLICATIONS IN HIGH SPEED CONTINUOUS CASTING OF BILLETS

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DISSERTATION

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To my parents.

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Abstract

Hot tear cracks and related defects are important issues that limit both productivity and quality of the continuous casting of steels. Computational models can play a crucial role for understanding and predicting these problems, and providing directions for improvements. Previous thermal stress models of the continuous casting process are reviewed, focusing on treatment of the mushy zone and hot-tear criteria. Existing hot-tear criteria are reviewed and evaluated. A two-phase (solid and liquid) model describing the mushy steel is developed as an initial step toward developing comprehensive hot tear criteria for steel casting. An empirical strain criterion is, then, chosen to predict hot tear cracks, based on thermal and stress histories.

A coupled finite-element model, CON2D, is improved to predict hot tear cracks based on the temperature and stress histories during the continuous casting of steel focusing on high speed billet casting. Thermal boundary conditions are investigated to make realistic predictions of high speed casting. These include heat flow at the strand surface, gap dependent thermal model across the interfacial layer between the mold and steel strand, and uneven superheat distribution at the solidification front due to the flow of liquid steel. A method based on a micro-segregation model is implemented to provide better liquid and solid phase fractions. A creep-based constitutive model is applied to treat liquid and mushy regions, rather than using a non-physical small elastic modulus as done in previous models. The empirical hot tear criterion is integrated into CON2D to predict hot tear cracks. The model is first validated by accurately matching an analytical solution for both temperature and stress in a solidifying slab with properly refined mesh and time step sizes. It is further validated by simulating continuous casting of a 120mm billet and compares favorably with plant measurements of mold wall temperature, total heat removal, shell thickness, including thinning of the corner and bulged shape.

The model is then applied to investigate three separate issues in high speed continuous casting. Firstly, the minimum shell thickness to avoid breakouts is predicted. Failure occurs

when the total strain across the local thin shell due to ferrostatic pressure exceeds the critical strain where hot tear cracks initiate. The predicted minimum shell thickness is only 3mm and varies slightly with steel carbon content. Without local thin spots, this restriction does not put practical limits on maximum casting speed. Considering that peritectic steels are more likely to have local thin spots, this explains their propensity for breakouts. Secondly, the maximum casting speed to avoid hot off-corner sub-surface cracks is predicted when the maximum accumulated damage strain exceeds the critical strain. This first occurs beneath off-corner surface. The predicted casting speed limit is up to 6.4m/min for a 120mm square billet casting in a 1100mm long mold. The limit drops with increasing section size and decreasing mold length. These predictions are confirmed by reported plant practice casting speeds. Thirdly, optimal mold taper is investigated along the casting direction with special attention to the corner effects. Simulation shows that the mold wall at the billet corner should not exactly follow the strand as commonly believed. Instead, a small, controlled amount of gap at the corner is preferred to produce uniform surface temperature in order to avoid both in-mold corner surface cracks and sub-mold off-corner sub-surface cracks.

Table of Contents

| | | | Page |
|---------|----------|---|------|
| List of | Figure | es | xi |
| List of | Tables | 5 | xvi |
| List of | Abbre | eviations | xvii |
| Chapte | er 1. In | ntroduction | 1 |
| 1.1 | Proces | s Review | 3 |
| 1.2 | Object | tive | 4 |
| 1.3 | Metho | dology | 5 |
| 1.4 | Figure | s and Tables | 7 |
| Chapte | er 2. L | iterature Survey | 9 |
| 2.1 | Therm | al-Mechanical Models of Continuous Casting of Steel | 9 |
| | 2.1.1 | Simulation Scope | 9 |
| | 2.1.2 | Mechanical Behavior of Steels | 11 |
| | 2.1.3 | Thermal and Mechanical Boundary Conditions | 12 |
| 2.2 | Hot Te | earing Criteria | 15 |
| | 2.2.1 | Criteria based on Solid Fracture Theories | 16 |
| | 2.2.2 | Critical Strain Criterion | 17 |
| | 2.2.3 | Liquid Feeding Theory | 18 |
| | 2.2.4 | RDG Hot Tear Criterion | 19 |
| 2.3 | Consti | tutive Models of Mushy and Liquid Steels | 22 |
| | 2.3.1 | Treatment of Liquid Steel | 22 |
| | 2.3.2 | Mechanical Behavior of Material in the Mushy State | 23 |
| 2.4 | Figure | s and Tables | 27 |
| Chapte | er 3. N | Iodeling of Semi-Solid Steel | 29 |
| 3.1 | Govern | ning Equations in Mushy Region | 29 |
| | 3.1.1 | Density Constitutive Equations | 29 |
| | 3.1.2 | Conservation of Mass and Momentum | 30 |
| | 3.1.3 | Momentum Balance | 33 |
| 3.2 | Consti | tutive Model in Mushy Region | 35 |
| | 3.2.1 | Elastic Constitutive Model | 35 |
| | 3.2.2 | Inelastic Constitutive Model | 36 |

| | 3.2.3 | Inelastic Constitutive Models for Different Regions in Mushy Zone 4 |
|--------|---------|---|
| | 3.2.4 | Discussion |
| 3.3 | Figure | s and Tables $\ldots \ldots 55$ |
| Chapte | er 4. N | fodel Description |
| 4.1 | Heat 7 | Transfer Model |
| 4.2 | Stress | Model |
| | 4.2.1 | Governing Equation |
| | 4.2.2 | Constitutive Equations |
| 4.3 | Finite | Element Implementation |
| | 4.3.1 | Heat Transfer and Solidification Model |
| | 4.3.2 | Stress Model |
| 4.4 | Numer | rical Integration Scheme |
| 4.5 | Treatn | nent of the Mold - Shell Interface |
| | 4.5.1 | Interface Heat Transfer |
| | 4.5.2 | Gap Size Calculation |
| | 4.5.3 | Thermal - Stress Coupling |
| 4.6 | Model | ing the Mold Wall |
| | 4.6.1 | Mold Wall Shape |
| | 4.6.2 | Contact Algorithm for Shell Surface Constraint |
| 4.7 | Solidif | ication Front Treatment |
| | 4.7.1 | Superheat Flux |
| | 4.7.2 | Ferrostatic Pressure |
| 4.8 | Impler | nentation of the Hot Tear Criterion under Complex Strain State 74 |
| | 4.8.1 | Hot Tear Criterion in CON2D |
| | 4.8.2 | Hot Tear Criterion in a 3-D Model |
| 4.9 | Mecha | nical Properties |
| | 4.9.1 | Phase Fraction Model |
| | 4.9.2 | Thermal Properties |
| | 4.9.3 | Thermal Linear Expansion |
| | 4.9.4 | Inelastic Constitutive Properties |
| | 4.9.5 | Elastic Properties |
| 4.10 | Model | Validation |
| 4.11 | Simula | ation of Billet Casting |
| 4.12 | Figure | s and Tables \ldots \ldots \ldots 39 |
| Chapte | er 5. C | ritical Shell Thickness Due to Tensile Rupture |

| 5.1 | Heat Flux Profile |
|--------|--|
| 5.2 | Materials Detail |
| 5.3 | Typical Results |
| 5.4 | Critical Shell Thickness |
| 5.5 | Critical Average Heat Flux in Mold |
| 5.6 | Implications |
| | 5.6.1 Casting Speed $\ldots \ldots 132$ |
| | 5.6.2 Depth of Oscillation Marks |
| 5.7 | Figures and Tables |
| Chapte | er 6. Billet Sub-Mold Bulging |
| 6.1 | Modeling Domain |
| 6.2 | Heat Flux Profile |
| 6.3 | Parametric Study and Computational Details |
| 6.4 | Typical Results |
| | 6.4.1 Heat Transfer Model Results |
| | 6.4.2 Stress Model Results |
| | 6.4.3 Failure Mechanism |
| | 6.4.4 Critical Casting Speed |
| | 6.4.5 Effect of Section Size and Mold Length |
| 6.5 | Implications |
| 6.6 | Figures and Tables |
| Chapte | er 7. Ideal Taper Prediction 169 |
| 7.1 | Heat Transfer Resistor Model $(0.75\% m^{-1} \text{ Taper}) \dots \dots$ |
| 7.2 | Uniform Heat Flux Around Mold Perimeter Model |
| 7.3 | Uniform Surface Temperature Around Mold Perimeter Model 171 |
| 7.4 | Secondary Cooling Pattern |
| 7.5 | Billet Behavior For Different Mold Configurations |
| | 7.5.1 Surface Temperature and Shell Growth |
| | 7.5.2 Sub-Mold Bulging and Longitudinal Off-corner Sub-Surface Cracks $.$ 173 |
| | 7.5.3 Transverse Corner Cracks |
| 7.6 | Optimal Taper Profiles Near Billet Corner |
| 7.7 | Optimal Taper Profiles |
| 7.8 | Figures and Tables |
| Chapte | er 8. Summary |

| 8.1 | Summa | ary of CON2D Improvement | 188 |
|--------|----------|--|-----|
| 8.2 | Summa | ary of CON2D Applications | 189 |
| | 8.2.1 | Critical Shell Thickness Due to Tensile Rupture | 189 |
| | 8.2.2 | Casting Speed Limit Due to Sub-mold Bulging | 190 |
| | 8.2.3 | Ideal Taper of Billet Casting | 191 |
| 8.3 | Future | Work | 192 |
| Appen | dix A. | Finite Element Implementation of the Heat Transfer Model | 195 |
| A.1 | Linear | Temperature Triangles | 195 |
| A.2 | Condu | ctance Matrix and Capacitance Matrix | 195 |
| Appen | dix B. | Finite Element Implementation of the Stress Model | 197 |
| B.1 | Linear | Strain Elements | 197 |
| B.2 | Genera | lized Plane Strain Formulation | 197 |
| B.3 | Global | Stiffness Matrix and Force Vectors | 199 |
| Appen | dix C. | Sweeping Algorithm | 200 |
| Refere | nces . | | 202 |
| Autho | r's Biog | graphy | 223 |

List of Figures

Page

| Fig. 1.1 Fig. 1.2 | Schematic overview of a two-strand slab casting process [1] | 7 8 |
|----------------------|--|----------|
| Fig. 2.1 | Sequence showing nucleation of a hot tear as two pores in an initially healed hot tear [3] | 27 |
| F1g. 2.2 | SEM image with close-ups of a torn-apart solidined bridge on a not tear surface in an Al-3wt.% Cu alloy showing a deformed surface structure on the main part of the spike and an undeformed draped-looking shape near | |
| | the root [3] | 28 |
| Fig. 3.1 | Volume of mass conservation | 53 |
| Fig. 3.2 | General material volume in mushy zone with both solid and liquid \ldots | 54 |
| Fig. 3.3 | Stress and strain within a material volume | 54 |
| Fig. 4.1 | Schematic of the modeling domain of casting billet | 93 |
| Fig. 4.2 | L-shape mesh with 3-node heat transfer and 6-node stress elements | 94 |
| Fig. 4.3 | Schematic of thermal resistor model of the interfacial layer between mold | |
| | and shell surface | 94 |
| Fig. 4.4 | CON2D flow chart | 95 |
| Fig. 4.5 | Three types of penetration modes in contact algorithm | 96 |
| Fig. 4.6 | Schematic of the moving front tracking method | 97 |
| Fig. 4.7 | Non-equilibrium Fe-C phase diagram predicted by the microsegregation model used in CON2D (other components: 1.52%Mn, 0.34%S, 0.02%S, | |
| | 0.012%P) | 97 |
| Fig. 4.8 | Evolution of the fractions of solid, δ -ferrite, and austenite from liquidus to solidus for the six carbon steels investigated in this work (other components) | |
| | 1.52% Mp. 0.34% S. 0.02% S. 0.012% P. | 08 |
| Fig 19 | Conductivity of plain carbon steels | 90 00 |
| Fig. 4.5 | Enthalpy of plain carbon steels | 100 |
| Fig. 4.10 | Thermal linear expansion (TLE) of plain carbon steels | 101 |
| Fig. 4.12 | Comparison of CON2D predicted and measured stress (Wrav) at 5% plastic | 101 |
| 8, -1, -2 | strain | 102 |
| Fig. 4.13 | CON2D prediction of the stress-strain relation of steel compared with mea- | |
| 00 | surements for uniaxial tensile test up to $1400 \ ^{o}C$ | 102 |

| Fig. 4.14 | CON2D prediction of the stress-strain relation of steel compared with mea- | |
|-----------|---|------|
| | surements for uniaxial tensile test above 1400 oC | 103 |
| Fig. 4.15 | CON2D prediction of the stress-strain relation of steel compared with mea- | |
| | surements for creep test at elevated temperature | 104 |
| Fig. 4.16 | CON2D prediction of the stress-strain relation of steel compared with cyclic | |
| | loading condition at elevated temperature | 105 |
| Fig. 4.17 | Elastic modulus for plain carbon steels used in CON2D | 106 |
| Fig. 4.18 | Temperature profiles through an infinite solidifying plate at different solid- | |
| | ification times comparing with Boley and Weiner analytical solution $\left[4\right]$ | 106 |
| Fig. 4.19 | Stress profiles through an infinite solidifying plate at different solidification | |
| | times comparing with Boley and Weiner analytical solution $[4]$ | 107 |
| Fig. 4.20 | Time step size effect to CON2D temperature prediction | 107 |
| Fig. 4.21 | Time step size effect to CON2D stress prediction | 108 |
| Fig. 4.22 | Mesh refinement effect to CON2D temperature prediction | 109 |
| Fig. 4.23 | Mesh refinement effect to CON2D stress prediction | 109 |
| Fig. 4.24 | Schematic of slice domain at the billet centerline | 110 |
| Fig. 4.25 | Superheat flux used in CON2D for billet casting simulation | 110 |
| Fig. 4.26 | Predicted instantaneous heat flux profiles in billet casting mold \ldots . | 111 |
| Fig. 4.27 | Predicted mold wall temperature profiles compared with plant measurement | s112 |
| Fig. 4.28 | Predicted shell thickness profiles for billet casting compared with plant | |
| | measurements | 113 |
| Fig. 4.29 | Mold distortion, mold wall position and shell surface profiles for the billet | |
| | casting simulation | 114 |
| Fig. 4.30 | Gap evolution predicted by CON2D for the billet casting simulation $\ . \ .$ | 115 |
| Fig. 4.31 | Shell surface temperatures predicted for billet casting simulation \ldots . | 116 |
| Fig. 4.32 | Temperature contours at 285mm below meniscus compared with corre- | |
| | sponding sulfur print from plant trial | 117 |
| Fig. 4.33 | Surface stress histories predicted near the billet face center (2-D L-mesh | |
| | domain) | 118 |
| Fig. 4.34 | Stress, temperature and strains predicted through the shell thickness far | |
| | from billet corner (slice domain) $\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$ | 119 |
| Fig. 4.35 | Stress predicted through the shell thickness near billet corner (2-D L-mesh | |
| | domain) | 120 |
| Fig. 4.36 | Stress contours predicted at mold exit | 121 |
| Fig. 4.37 | Inelastic strain contours predicted at mold exit | 122 |

| Fig. 5.1 | Slice model domain with finite element mesh and region of shell modeled . | 135 |
|-----------|---|------|
| Fig. 5.2 | Average heat flux with respect to contact time (A - [5], B - [6], C - [7], D | |
| | - [8]) | 136 |
| Fig. 5.3 | Instantaneous heat flux with respect to distance below meniscus casting at | |
| | 2.2m/min(Total heat is for a 1100mm mold) | 136 |
| Fig. 5.4 | Typical thermal-mechanical histories at strand surface $(0.044\% C \text{ carbon})$ | |
| | steel cast in 200mm square, $800mm$ long mold at $1.0m/min$) | 137 |
| Fig. 5.5 | Temperature and stress distribution through the solidifying shell (0.044% C | |
| | carbon steel cast in 200mm square, 800mm long mold at $1.0m/min)$ | 138 |
| Fig. 5.6 | Oscillation mark depth for steels with different carbon content $[9]$ | 138 |
| Fig. 5.7 | Carbon content effect on critical shell thickness $(200mm \text{ square bloom},$ | |
| | $800mm \text{ mold}) \dots \dots \dots \dots \dots \dots \dots \dots \dots $ | 139 |
| Fig. 5.8 | Super heat effect on critical shell thickness (0.044% C steel cast in $200mm$ | |
| | square bloom, $800mm$ long mold) $\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$ | 140 |
| Fig. 5.9 | Section size effect on critical shell thickness (0.044% C steel cast in $800mm$ | |
| | $long mold) \dots \dots \dots \dots \dots \dots \dots \dots \dots $ | 140 |
| Fig. 5.10 | Working mold length effect on critical shell thickness (0.044% C steel cast | |
| | in 200 mm bloom) \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots | 141 |
| Fig. 5.11 | Effect of total heat removed by mold and section size on total strain | |
| | $(0.044\% C \text{ steel at } \dot{\epsilon} = 10^{-3} sec^{-1}) \dots \dots$ | 141 |
| Fig. 5.12 | Heat flux extracted by mold casting at $2.2m/min$ - influencing factors $~$ | 142 |
| Fig. 5.13 | Critical casting speed - influencing factors | 142 |
| Fig. 5.14 | Heat flux in mold as a function of oscillation mark depth $[9]$ | 143 |
| Fig. 5.15 | Critical oscillation mark depths at $2.2m/min$ - influencing factors | 143 |
| Fig. 6.1 | Measured average heat flux and fitted average heat flux curve | 154 |
| Fig. 6.2 | Instantaneous heat flux curve | 155 |
| Fig. 6.3 | Shell thickness history (Section size: $120mm$, working mold length: $700mm$ |)155 |
| Fig. 6.4 | Surface temperatures history (Section size: $120mm$, working mold length: | |
| | 700mm) | 156 |
| Fig. 6.5 | Surface temperature at mold exit and below (Section size: $120mm$, working | |
| | mold length: $700mm$) | 157 |
| Fig. 6.6 | Distorted temperature contour at mold exit (Section size: $120mm$, working | |
| | mold length: $700mm$) | 158 |
| Fig. 6.7 | Hoop stress contours (Section size: $120mm$, working mold length: $700mm$) | 159 |

| Fig. 6.8 | Hoop total strain contours (Section size: $120mm$, working mold length: $700mm$) | 160 |
|-----------|---|-----|
| Fig. 6.9 | Continuous-cast billet section after breakout showing off-corner subsurface crack | 161 |
| Fig. 6.10 | Surface displacements at mold exit and $200mm$ below (Section size: $120mm$, working mold length: $700mm$) | 161 |
| Fig. 6.11 | Histories of strains at $(6.7mm, 17.4mm)$ (Section size: $120mm$, working mold length: $700mm$, Speed: $2.2m/min$) | 162 |
| Fig. 6.12 | Histories of strains at $(6.7mm, 17.4mm)$ (Section size: $120mm$, working mold length: $700mm$, speed: $5.0m/min$) | 163 |
| Fig. 6.13 | Stress along casting direction (Z direction) at mold exit (Section size: $120mm$, working mold length: $700mm$) | 163 |
| Fig. 6.14 | Hoop damage strain (Section size: $120mm$, working mold length: $700mm$) | 164 |
| Fig. 6.15 | Z damage strain at mold exit (Section size: $120mm$, working mold length: $700mm$) | 164 |
| Fig. 6.16 | Displacement histories at surface center (Section size: $120mm$, working mold length: $700mm$) | 165 |
| Fig. 6.17 | Maximum bulging vs. casting speeds | 165 |
| Fig. 6.18 | CON2D predicted critical casting speeds and corrected critical speeds ac- counted partial mold end support | 166 |
| Fig. 6.19 | Comparison of the critical speeds based on hot-tear criterion and typical plant practice [10] | 166 |
| Fig. 6.20 | Comparison of the critical speeds based on 1mm maximum bulging criterion and typical plant practice [10] | 167 |
| Fig. 7.1 | Mold distortion for 2-D simulation | 178 |
| Fig. 7.2 | Measured average heat flux and fitted functions | 179 |
| Fig. 7.3 | Instantaneous heat flux curve | 179 |
| Fig. 7.4 | Uniform surface temperature | 180 |
| Fig. 7.5 | Heat transfer coefficient in spray zone | 180 |
| Fig. 7.6 | Temperature contours at the mold exit | 181 |
| Fig. 7.7 | Surface temperature histories casting at $2.2m/min$ for three mold configu- rations | 182 |
| Fig. 7.8 | Stress contours at $100mm$ below mold exit casting in the $0.75\%m^{-1}$ linear | |
| | taper mold (inadequate taper) | 182 |

| Fig. 7.9 | Damage strain contours at $100mm$ below mold exit casting in the $0.75\%m^{-1}$ | |
|-----------|---|-----|
| | linear taper mold (inadequate taper) | 183 |
| Fig. 7.10 | Axial stress contours at $100mm$ below mold exit casting in the mold with | |
| | too much taper | 184 |
| Fig. 7.11 | Axial stress contours in the mold with too much taper | 184 |
| Fig. 7.12 | Shell shrinkage, heat flux and gap at the mold exit casting at $2.2m/min$ | |
| | with the ideal mold taper (uniform surface temperature) | 185 |
| Fig. 7.13 | Optimal taper prediction | 185 |
| Fig. 7.14 | Optimal taper profiles predicted by slice model | 186 |
| Fig. 7.15 | Shrinkage at $1000mm$ | 186 |
| Fig. 7.16 | Shrinkage at mold exit vs. total heat extracted by mold | 187 |
| Fig. 7.17 | Maximum mold distortion vs. average heat flux | 187 |
| Fig. A.1 | Six-node quadratic displacement triangle element with Gauss points for | |
| | stress model with corresponding four three-node linear temperature triangle | |
| | elements for heat flow model | 196 |
| Fig. C.1 | Sweeping algorithm | 201 |

List of Tables

| Table 4.1 | Parameters in the heat resistor model | 23 |
|-----------|---|----|
| Table 4.2 | Value of the parameters in enthalpy equation 4.56 | 23 |
| Table 4.3 | Carbon content function in the enthalpy equation 4.56 | 23 |
| Table 4.4 | Constants used in Boley and Weiner analytical solution | 24 |
| Table 4.5 | Material details in billet plant trial at POSCO | 25 |
| Table 4.6 | Simulation conditions in billet plant trial at POSCO | 25 |
| | | |
| Table 5.1 | Solidus and liquidus temperatures and critical strain | 14 |
| Table 5.2 | Casting conditions for practice shown in Figure 5.14 for $0.27\%\mathrm{C}$ steel casting 14 | 14 |
| | | |
| Table 6.1 | Parametric study conditions | 38 |
| Table 6.2 | Steel compositions and important transforming temperatures | 38 |
| Table 6.3 | Critical strains (%) $\ldots \ldots \ldots$ | 38 |
| Table 6.4 | Productivity limits $(tonnemin^{-1})$ 16 | 38 |
| | | |

List of Abbreviations

- ALE Arbitrary Lagrangian Eulerian approach.
- LHS Left Hand Side.
- **LIT** Liquid Impenetrable Temperature. The temperature where the fraction of solid is high enough to stop liquid feeding.
- **RHS** Right Hand Side.
- **ZDT** Zero Ductility Temperature. The temperature where the fraction of liquid is high enough to make semi-solid material loose its ductility.
- **ZST** Zero Strength Temperature. The temperature where the fraction of liquid is high enough to make semi-solid material lose mechanical strength.

Chapter 1. Introduction

Continuous casting has been producing semi-finished steel shapes: blooms, billets, slabs and strips, with increasing high quality at lowering cost since it is introduced in 1964 [11]. The process, as shown in Figure 1.1 as a typical two strand slab casting, has been adopted worldwide by the steel industry. By 2002, the crude steel output from the continuously cast process is more than 88% of the total world steel production of 794.5 million metric tons [12].

As the steel industry continues to improve quality and reduce cost, there is growing interest in maximizing the productivity from a single continuous casting machine. Many different processes are currently competing, from conventional thick slab and blooms to thin slabs and strip casting, whose economic feasibility depends on their eventual productivity. Considering the high cost of plant experiments, it is appropriate to apply computational modeling to explore the theoretical limits of continuous casting speed and productivity.

Productivity increases with increasing casting speed and increasing cross-section area. The casting speed is limited by several different phenomena, listed below.

- Excessive level fluctuations and waves at the meniscus become worse with greater casting speed. This can cause surface quality problems and even sticker "breakouts". This problem can be addressed by changing nozzle design (directing the flow more downward, possibly by adding a bottom vertical port), applying electromagnetic forces, changing mold fluxes, and using other methods to control the flow pattern in the mold.
- 2. Excessive axial strains caused by the oscillation and withdrawal forces needed to overcome friction between the solidifying shell and the interfacial layers in the mold can lead to transverse cracks and breakouts at mold exit. Schwerdtfeger [7] has calculated that these stresses are negligible if the liquid layer of the mold flux can be kept continuous over the entire mold surface.

- 3. Excessive transverse strains may be generated in the thin shell by the ferrostatic pressure of the liquid pool below the mold. This can lead to longitudinal cracks and "breakouts" if the shell is not thick enough at mold exit.
- 4. Any local nonuniformity in the shell growth can lead to locally hot and thin regions in the shell, which can initiate longitudinal cracks and breakouts even if the shell is above the critical thickness on average. This problem, which has been investigated by Brimacombe and others, [13] can be addressed by optimizing mold flux behavior during initial solidification, oscillation practice, and taper design, such that flux lubrication is continuous, the initial heat flux is low and uniform, and the mold wall taper matches the shell shrinkage profile [14]. Peritectic steel grades and austenitic stainless steel are most susceptible to this problem. Superheat delivered from the flowing steel jets can also contribute to this problem, especially near the narrow faces in slab casting with bifurcated nozzles.
- 5. Excessive bulging of the strand below the mold can lead to a variety of internal cracks and even breakouts if the bulging is extreme. Bulging can be controlled by choosing short enough support roll spacing, maintaining roll alignment, controlling spray cooling below the mold, and by avoiding sudden changes in roll pitch, sprays, or casting speed.
- 6. The distance below the meniscus of the point of final solidification of the center of the strand increases in direct proportion with casting speed for a given section thickness, which usually limits the maximum casting speed in a given steel plant. The torch cut-off, spray cooling system, and roll support system all must extend to accommodate this increase in metallurgical length. Contrary to intuition, this metallurgical length cannot be significantly shortened by increasing the spray cooling intensity [15]. This understanding is incorporated in the pioneering work of Brimacombe and coworkers to provide design criteria for spray zones [15, 16].

7. Finally, there are many other special quality concerns which sometimes impose limits on casting speed. For example, in ultra-low carbon steels, a relatively slow upper limit in casting speed is required in order to reduce pencil pipe and other blister defects due to argon bubble entrapment on the inner radius of curved mold casters [17, 18]. Casting speed can only be increased in these situations by careful changes in operating conditions that avoid the specific defects of concern.

The capability of making high quality and low cost steel by the continuous casting process is limited by these and other problems. These defects result in tons of scrapped product annually, expensive defect detection equipment, and other efforts that increase the cost for the steel producing companies, and ultimately the consumer. Several physical phenomena, such as the chemical reactions among steel compositions, flow pattern of the liquid steel, heat transfer, solidification as well as the evolution of residual stresses etc., compete with each other during the process and control the behavior of the steel. The complicated nature of the process and the harsh operating conditions make it very difficult to simulate the process in experiments under realistic condition. This makes mathematical simulation an important tool to gain insight into the process.

1.1 Process Review

A schematic representation of the continuous casting process is shown in Figure 1.2 focusing on the mold region. The superheated liquid steel is poured into the open ended water cooled copper mold through a nozzle, that is submerged into the liquid steel pool. Heat is extracted from the liquid steel by the cooling water flowing through the mold water slots across the partially solidified steel shell, the interfacial layer between the shell surface and the mold wall, and the copper mold wall. The steel shell keeps growing as it is pulled down the mold and builds up enough thickness and strength to withstand the ferrostatic pressure from the liquid steel due to gravity until it reaches the mold exit. The mold is tapered to

follow the shrinkage of the steel shell and distorted due to the temperature gradients that develop where the mold wall does not follow the shell shrinkage perfectly, gaps may form between the mold wall and shell surface, which reduce the heat transfer rate and leads to local hot spots on the shell. In extreme situations, liquid steel will break through the hot and weak shell, which is commonly referred to as a "breakout". The mold oscillates during operation to prevent the shell from sticking to the mold wall. This allows the shell to be withdrawn out of the mold without tearing. The oscillation is also responsible for transverse ripples, called "oscillation marks" on the strand surface which will influence the heat transfer rate between the mold wall and the strand surface.

Below the mold exit, the shell is pushed outward due to the ferrostatic pressure from the liquid pool, causing "bulging" as shown in Figure 1.2. Bulging results stresses in the solidifying steel shell and leads to longitudinal surface cracks at the strand face center and subsurface creates near the corner. The amount of bulging is directly related to the the thickness of the steel shell and further related to other operation conditions such as casting speed and super heat, and mold conditions such as mold dimensions and taper.

The shell is further cooled by water sprays and passes a series of the guide rollers in an arc, which is to reduce the height of the caster, until it travels horizontally as shown in Figure 1.1. The strand length from the meniscus to the position where the strand is totally solidified is termed the "metallurgical length". Then, the completely solidified product is torch-cut into final slabs of desired length. The section shape of the final slab is normally not the same as the section shape of the mold, which is called shape distortion, due to residual stresses during the solidification and the cooling procedure.

1.2 Objective

The objective of this work is to investigate 3 different practical continuous casting problems, including critical shell thickness due to membrane stress caused by ferrostatic pressure, casting speed limit due to sub-mold bulging, and ideal taper prediction, by using the thermalmechanical finite element model, CON2D, which was previously developed by professor Brian G. Thomas and his students [19, 20]. Further development work is needed as part of this project to make the model more accurate and to verify this accuracy. These include implementation of a non-equilibrium phase diagram for improving property prediction for plain carbon steels, improvement of the heat transfer model to better incorporate mold flux and the mold wall into the model, improvement of the stress model to treat liquid and mushy elements more accurately, and adding a fracture criterion into the model to predict cracking tendency near the solidification front.

1.3 Methodology

To achieve these objectives, the following is performed which is described in this thesis:

In Chapter 2, previous work on the development of mathematical models for the continuous casting process is reviewed. These includes the modeling scope, the numerical methodology, the steel behavior at elevated temperatures, and the temperature dependent properties. Then, previous hot tear criteria are reviewed and evaluated. A strain criterion [21] is chosen to implement in CON2D to predict hot tear cracks quantitatively. At last, several constitutive models for the mushy region are reviewed because it is very important to model this region reasonably to make it possible to predict hot tear cracks, which is well believed to initiate here.

In Chapter 3, the mechanical behavior of the mushy region is investigated using spatial averaged governing equations (mass and momentum balance equations for single phase liquid and solid steels) over a small control volume contains both liquid and solid phases. Constitutive models are proposed for mushy regions with different solid fractions.

In Chapter 4, the in-house developed 2-D finite element thermal mechanical model under the generalized plane strain assumption, CON2D, is introduced in detail. This model features elastic-viscoplastic constitutive models for δ -, α -ferrite, and austenite(γ). A creep-dependent function is applied to grasp the liquid behavior properly. An efficient alternating implicitexplicit numerical integration method solves this highly non-linear problem. A specially designed contact algorithm, a moving internal boundary tracking method, as well as an interfacial heat resistor model fully coupling the heat transfer and the stress models model the continuous casting process as realistic as possible. Other features such as uneven super heat distribution according to fluid flow model, and temperature dependent steel properties are also included in CON2D. Finally, the model is validated against both analytical solution and plant measurements from industry.

Chapter 5 investigates the critical thickness necessary to contain the liquid pool and avoid longitudinal rupture or "breakouts" due to excessive creep strain of the thin shell. This investigates the minimum total heat necessary to be extracted by mold to generate thick enough shell to avoid cracks , and further leads theoretical upper limits on casting speed and local gap sizes imposed by this need.

Chapter 6 focuses on quantifying the effect of sub-mold bulging to the initiation of offcorner sub-surface hot tearing cracks by applying CON2D to predict temperature, bulging, strain, stress and fracture in billets, in the absence of any sub-mould support. The results are then used to find the critical casting speeds to avoid quality problems related to bulging below the mold as a function of section size and mould length.

The criteria for how to chose optimal taper is studied in this work in chapter 7, based on simulations of the thermal-mechanical behavior of billets with the three types of mold configuration producing hot corner, cold corner and equal surface temperature around the perimeter. Optimal taper profiles are then predicted as a function of casting speed, using a computational model fit to match billet heat flux measurements.

In Chapter 8, conclusions and some recommendations for the future advance are drawn.

1.4 Figures and Tables



Fig. 1.1: Schematic overview of a two-strand slab casting process [1]



Fig. 1.2: Schematic of continuous casting process (not to scale) [2]

Chapter 2. Literature Survey

2.1 Thermal-Mechanical Models of Continuous Casting of Steel

Thermal-mechanical modeling is an important tool to assist people understanding the fundamentals of quality issues such as cracks and shape distortions owing to the residual stresses and strains generated by thermal and mechanical loads. Previous literature is reviewed in this chapter according to their consideration of the following crucial aspects.

- 1. Properly chosen simulation scope.
- 2. Realistic thermal and mechanical properties of steels at elevated temperatures.
- 3. Reasonable mechanical behavior function of steels at elevated temperatures.
- 4. Adequate treatment of thermal and mechanical boundary conditions at the surface and solidification front of the solidifying steel.

Even though the computing power of modern computers is increasing at a tremendous speed, it is still far from satisfying the demands of a complex model having all of the realistic features listed above. Moreover, some of the features, such as physical properties and mechanical behavior of steels, are not well defined especially near the solidus and liquidus temperatures. Therefore, all existing models are subject to some simplifications from reality which lead to different approaches.

2.1.1 Simulation Scope

Skipping the design details, the continuous casting process is nothing but pouring liquid steel into an open mold and dragging the solidified steel out of the bottom. During most time of the operation, continuous casting process is in steady state, neglecting some transient phenomena such as process start-up, meniscus fluctuation and mold oscillation. This makes Eulerian approach based on spacial frame of reference a natural choice for many practical problems. However, the mechanical behavior of steels at elevated temperature range of the continuous casting process is highly inelastic and history dependent. The temperature, stress, and strain states are associated with the material points and their state history. This makes a Lagrangian approach which tracks a portion of steel from the meniscus be a better candidate.

Even though both approaches have been adopted depending on different applications, the Lagrangian approach is more favorable due to its ease of implementation. Many researchers developed their models using a Lagrangian frame tracking a portion of steel (1D slice, 2D section slice, 2D longitudinal slice or 3D blocks) from the meniscus. These include early models back to the late 1970s and early 1980s by Brimacombe and his colleagues [22-25], Rammerstorfer et. al. [26–29], Kristiansson et. al. [30–32], Kinoshita et. al. [33] as well as recent models by Thomas and his colleagues [34–38], Park et. al. [39–41], Tszeng et. al. [42], Mizoguchi et. al. [43], Boehmer et. al. [44–47] and Han et. al. [48]. On the other hand, models based on an Eulerian approach have had limited implementation since the constitutive behavior is still based on materials points even though the modeling domain is associated with spatial points. In this approach, a special treatment is needed to take care of the advection term while integrating the constitutive equations on the material points moving relative to the spatial framework. Barber et. al. [49] and L. Yu [50] used this approach to investigate the bulging between two adjacent rolls. Kelly et. al. [51], Tatsumi et. al. [52], and Lee et. al. [53] used their models to simulate the mold and shell interactions as the steel flow through the mold. A model based on a new method called Arbitrary Lagrangian Eulerian (ALE), which is an extension of the Eulerian approach, is developed by Fachinotti et. al. [54, 55] and used to predict the gap between the mold and the shell surface for round billet casting.

Fachinotti *et. al.* claimed that the Eulerian approach has an accuracy advantage [56] over a Lagrangian approach that models only a slice of steel, especially for simulating mold and shell interactions to predict the gap. This is because the Lagrangian approach with a

slice section domain assumes independence between the slices at different distances below meniscus. However, the computing capability of modern computers is still not enough to perform accurate 3D simulations with either Lagrangian or Eulerian approaches with a properly refined mesh and realistic material behavior in a feasible time frame. Therefore, most of the models used to gain realistic and practical insight in slab and square billet casting only have a 2D modeling domain under either axi-symmetric [51–53] or plane stress/strain assumptions [22–41]. In this situation, the Lagrangian approach is able to model almost all continuous casting stand shapes, billets, blooms, slabs, and even strips, while the Eulerian approach is limited to round blooms [51–55].

2.1.2 Mechanical Behavior of Steels

The mechanical behavior of steel, is the most important factor leading to a successful thermal mechanical simulation. Steels behave quite differently at elevated temperatures near their melting point. History-independent plasticity and history-dependent creep are too substantial to be neglected. Moreover, they cannot be distinguished during a tensile or compression test at elevated temperature [57]. Although many efforts have been made to investigate the mechanical behavior of steels near their melting temperature, including uniaxial tensile tests [58–61], creep tests [62], and bending tests [63], the actual behavior is still not fully quantified under all of the practical conditions experienced during the continuous casting of steel owing to its being highly history-dependent. Several types of constitutive models are used to model the mechanical behavior of steels at elevated temperatures close to their solidus temperature, including elastic-plastic models, elastic-creep models, elasticplastic-creep models and unified elastic-viscoplastic models.

The simple elastic-plastic models with an elastic modulus and one or more plastic moduli are applied to simulate the mechanical behavior of steel in some early stress models for the continuous casting process [22, 23, 25]. This model is improved to incorporate temperature dependent elastic and plastic moduli to capture more realistic steel behavior [45, 46, 51, 52]. These simple models are too crude to capture the steel behavior quantitatively. They could only provide qualitative understanding of the steel behavior. The loading conditions defined in the standard tensile test can be used to calibrate these elastic-plastic constitutive models. Specifically, the strain rate is chosen to match the actual process conditions.

The elastic-plastic approach neglects time dependency of the steel caused by creep, which is substantial at elevated temperature where the continuous casting process works. Some models, including elastic-creep and elastic-plastic-creep models, include creep to get more accurate steel behavior [27, 28, 30–32, 44, 47]. These models treat the creep and plasticity separately. Splitting the inelastic strain into a rate-independent plastic part and a ratedependent creep part is physically arbitrary, since both phenomena happen simultaneously during the tensile or creep experiment at the elevated temperature. It is difficult to find a set of elastic-plastic and creep model to accurately simulate the steel behavior.

Many recent stress models adopt "unified" elastic-viscoplastic constitutive equations with evolving internal structure variables such as stress, strain, and temperature [41,42,48,53,64]. In these models, the inelastic strain rate is a function of the current stress, inelastic strain, temperature. Some models [34–38,54,55,65] adopted a unified model with an extra state variable, steel carbon content, proposed by Kozlowski [66]. Integrating these equations under proper boundary conditions produces realistic stress-strain curves under arbitrarily chosen loading conditions. It could accurately simulate the steel behavior by considering these structure variables. However, the unified model is numerically too stiff to easily integrate. More advanced and robust integration algorithms and longer computational times are normally required. A review of numerical integration schemes for constitutive models can be found by Zhu [20].

2.1.3 Thermal and Mechanical Boundary Conditions

Besides the conventional boundary conditions of the thermal and stress models (specified temperature, heat convection coefficient, heat flux, fixed displacement, and surface traction)

several special boundary conditions are necessary to simulate the continuous casting process properly. Solidification and interaction between the mold wall and the shell each require special boundary models.

Interaction between the mold wall and the strand surface

Interactions between the mold wall and the strand surface include the heat transfer rate dependence on the gap between the mold and strand and the mechanical constraint of the mold to the strand. These two separate but related interactions often require the heat transfer model to be fully coupled with the stress model.

The heat transfer rate is a strong function of the gap formed between the mold Gap and the steel strand. Many efforts have been conducted to predict the ideal mold shape that can follow the strand shrinkage exactly to prevent the gap formation [34, 35, 67–71]. However, the gap cannot be totally eliminated because of the complicated 3-D profile of the shrinking strand surface. Moreover, the gap size depends greatly on the specific operation conditions of the caster and the type of steel being cast. Therefore, to model the heat transfer rate as a function of the gap yields more insight than providing a pre-described heat flow rate at the strand surface. Unfortunately, fully coupled models always lead to extra computational cost and the convergence difficulty, which makes the simulation take longer than an uncoupled one [44]. Many previous models included the interaction between the heat transfer and the stress models to determine the interfacial heat transfer rate during the analysis [32,33,36,41,45,47,48,51,53,54]. To solve this coupled problem, first the temperature field in strand is calculated using an estimation of the gap size between the strand surface and the mold wall. The stress model is then solved to get the shrinkage of the strand. The gap size is calculated from the strand shrinkage and the mold wall position. Finally, the gap sizes between each two consecutive iterations are checked until convergence is achieved.

Some models also calculate the temperature field in the mold to give an accurate estimation of the mold distortion [41, 45, 48, 51, 53, 54].

Contact The mechanical constraint from the mold wall to the strand brings a high nonlinearity into the stress model as the strand could shrink freely away from the mold wall, but could not penetrate it when the strand contacts the mold wall. In a transient problem, the contact region and the contact pressure are both unknown a priori. Three main approaches, the Lagrange multiplier method [72–74], the penalty method [75, 76], and the augmented Lagrangian method [77–79], have been adopted for numerical treatment of contact in the context of finite-element methods. The penalty method approximately constrains the strand surface at the mold wall position by adding a very large number on the main diagonal terms of the stiffness matrix as if adding a very stiff spring between the mold wall and the strand surface. It is easy to implement with a little cost of accuracy. The Lagrangian methods introduce new unknowns, which represent the contact pressure, into the system. They can provide both constraint and contact pressure. However, they are difficult to implement and converge. Moreover, their computational cost are usually huge for large problems.

Moving Boundary - Solidification Front

The thermal stress model with solidification phenomena has a moving boundary - the solidification front. This moving front, identified by an isotherm, distinguishes how an element behaves, as solid or liquid.

From the heat transfer point of the view, the superheat contained in the liquid steel is distributed to the solidification front as the liquid flows around in the liquid pool. Some efforts have been made to include this by solving a fully coupled thermal-fluid-mechanical system simultaneously. It is no surprise that these models are very computationally expensive and difficult to develop. Kelly *et. al.* transferred data between two commercial packages, FIDAP and NIKE2D, to solve the coupled thermal-fluid-mechanical model to simulate the continuous casting of round billets [51]. Recently, Lee *et. al.* developed an integrated thermal-fluid-mechanical package to simulate continuous round billet casting [53]. Another way to incorporate this convective heat transfer due to fluid flow is to simulate the effect of the fluid flow pattern on the superheat distribution by a separate fluid flow model, and then input it as an internal boundary condition into the thermal-stress model [80].

From the stress point of view, the ferrostatic pressure from the liquid steel due to gravity acts on the solidification front pushing the solid shell toward the mold wall. Although a couple of models treated this in a natural way as a body force [45,54], many other models treat it as an internal boundary condition [31,32,36,41,47,48,51,53]. This is because the shear stresses of liquid steel is negligible compared to the shear stresses of solid steel. Therefore, the stress state in liquid is always hydrostatic pressure, considering that the liquid velocity is small under the normal conditions of the continuous casting of steel. It is an obvious advantage to apply the liquid pressure at the solidification front without solving the stress state in the liquid in stress model. Moreover, the effect of the gravity to the stress state in solid is always neglected. Then, the body force term is omitted to make the force balance equation simpler.

2.2 Hot Tearing Criteria

Hot tear cracking is a common problem encountered during the casting of alloys with large freezing range including steel. Over the last several decades, much effort has been put into the understanding of the hot tearing mechanisms [3, 81–86] and the predicting of hot tearing tendency in a quantitative manner [21, 87–90].

Hot tearing is a complex phenomenon which is due to uneven temperature distribution of the solidifying alloys and involves deformation of the coherent and non-coherent solid skeleton as well as flow of the interdendritic liquid. Since the later thermal-mechanical aspects are caused by solidification, many early hot tearing criteria simply consider the solidification interval of the alloy: the larger the freezing range, the more susceptible the alloy will be to hot tearing [91]. This obviously does not satisfy the need to predict hot tearing cracks accurately. Some recent studies on the hot tearing crack surfaces by Scanning Electron Microscopy (SEM) [3,86,91,92] have confirmed that both the pore nucleation due to insufficient liquid feeding of the interdendritic space and the solid fracture of the solid skeleton contribute to the formation of hot tears. Figure 2.1 and 2.2, taken from the work of Farup *et. al.* [3], show the initiation of a hot tear due to pore nucleation and the fracture of the solid skeleton, respectively. Hot tears in steel are inter-granular usually along prior austenite (γ) grain boundaries.

Several hot tearing criteria, including solid fracture theories and liquid filling theories, are proposed based on the understanding of the mechanism of hot tearing.

2.2.1 Criteria based on Solid Fracture Theories

These criteria are based on continuum mechanics theories assuming the hot tearing will occur at a critical stress [30, 33, 63, 93, 94] or strain in the mushy zone [21, 24, 82, 92, 95–97]. These theories are also used to predict solid fractures. Based on the chosen criteria, these theories can further break down into categories using a strain criterion, or stress criterion.

Strain criterion theories claim that hot tear cracks appear when the strain of the specific area exceeds the critical strain. Critical strains are measured by bending tests [98–104], punch press tests [95,97,105], and in-situ melt bending tests [106]. All these tests measure the critical strain at the solidification front when hot tear cracks initiate.

Stress criterion theories claim that hot tear cracks appear when the stress of the specific area exceeds the critical stress value. Like the critical strain, the critical stress can also be obtained from mechanical tests of the alloys higher than their solidus temperature. These tests include submerged split chill tensile tests [107, 108], tensile tests [109–112] and compression tests [113].

These empirical criteria are able to reflect realistic conditions and be very simple to implement into stress models. However, they strongly depend on the experiment conditions, such as the temperature and the loading histories, as well as the compositions of the tested steels. Therefore, they cannot necessarily be applied to general cases.

2.2.2 Critical Strain Criterion

A hot tearing crack criterion which is the best strain criterion available from the existing literature found by author is judged to be by WON [21] and fitted from the data from 37 experiments [98,99,101–103] as a function of strain rate, $\dot{\epsilon}$ (sec.⁻¹), and brittle temperature range, ΔT_B (°C), within which liquid feeding is terminated by the coherent dendrites, as given in Equation 2.1.

$$\epsilon_c(m/m) = \frac{0.02821}{(\dot{\epsilon}(sec.^{-1}))^{0.3131} (\Delta T_B(^oC))^{0.8638}}$$
(2.1)

This simple empirical equation represents a great deal of experimental efforts at the elevated temperatures near the solidification temperatures of plain carbon steels. These experiments bend as-cast slabs containing liquid core in a 3-point bend test at controlled strain rate ($\sim 1 \times 10^{-3} sec.^{-1}$). The total strain near the solidification front is calculated from the pushing distance of the punch head and the curvature of the slab surface. This criterion takes into account the effects of brittle temperature range, which is defined between the temperatures when the solid fraction is between 90% and 99% and the average strain rate within ΔT_B . It is seen that larger brittle temperature range and strain rate lead to smaller critical strain which implies easiness of crack initiation. The brittle temperature range includes the effects of the chemical compositions and the cooling rate, and the strain rate reflects the external loading conditions. The trend is the same as those more sophisticated theories discussed next. Therefore, this criterion, although very simple, is a good candidate to predict hot tear cracks quantitatively under realistic conditions.

Equation 2.1 is far from ideal due to its empirical nature. It incorporates the effects of loading conditions, cooling rates, chemical compositions, micro- and macro-segregation, and

microstructure of the carbon steel to the formation of hot tear cracks through two physical variables, strain rate and brittle temperature range. As a consequence, the application of this equation is limited to those steel casting processes with similar operation conditions as those during the experiments and the units of the two physical variables have to be the same as those mentioned in Equation 2.1. It is desirable if this equation could be made dimensionless by fundamental-based dimensional analysis that includes the other physical variables, such as cooling rate, concentration of chemical compositions, primary and/or secondary dendrite arm spacings and etc., directly into the equation. This is not a trivial task within the scope of this work. The development of the more comprehensive hot tear criterion is included in the recommended future work in Section 8.3 of Chapter 8.

2.2.3 Liquid Feeding Theory

These theories assume that the hot tear forms due to a lack of liquid feeding into the mushy region. As liquid flowing through the mushy region, the pressure of the liquid drops. Pores will nucleate as the pressure of the liquid drops below the critical pressure of the solute gas components. Fluid flow in the interdendritic region can be modelled by Darcy's Law:

$$\boldsymbol{v} = -\frac{K}{\mu} \nabla p \tag{2.2}$$

where \boldsymbol{v} , K, and p are the velocity vector of the liquid, the permeability of the solid skeleton, and liquid pressure, respectively.

Niyama [114] proposed a hot tear model based on the assumption that a hot tear initiates when a cavity is nucleated in the liquid. The mushy zone deformation decomposes into two components, the solid and the liquid deformations. The solid is assumed to follow power law, while the liquid stress is calculated according to its ability to flow into the expanding 1-D channel along y direction,

$$\sigma = \frac{2\mu l^2}{y^3} \frac{dy}{dt} \tag{2.3}$$

where $\mu(Pa \cdot s)$ is the viscosity of the liquid alloy, l(m) is the length of the mushy zone, and y(m) is the primary dendrite arm spacing. The mushy zone deformation velocity, $\frac{dy}{dt}$, represents the interdendritic flow speed $(m \cdot s^{-1})$. Equation 2.3 indicates the longer the mushy zone and the smaller the primary dendrite arm spacing, the larger stress is produced under a constant deformation rate. For an alloy whose mushy zone length, l, and primary dendrite arm spacing, y, are roughly fixed, hot tear cracks are assumed to initiate when the stress of mushy zone is large enough to initiate a spherical bubble. The critical strain rate when hot tear cracks form given below is calculated where a spherical pore of diameter y can be formed.

$$\dot{\epsilon}(s^{-1}) = 16 \left(\frac{k^2 \gamma^9}{\mu^3 l^6 L^3}\right)^{0.2} \tag{2.4}$$

where $k(N^{-3} \cdot s^{-1})$ is the creep law constant of the solid, $\dot{\epsilon} = k\sigma^3$, $\gamma(N \cdot m^{-1})$ is the surface energy of the alloy liquid, $\mu(Pa \cdot s)$ is the dynamic viscosity, l(m) is the thickness of the mushy zone, and L(m) is the primary dendrite arm spacing.

Feurer [115] proposed another theory assuming hot tear cracks happen when volumetric shrinkage rate due to solidification exceeds the volumetric liquid feeding rate. Volumetric shrinkage rate is calculated by,

$$\frac{\partial lnV}{\partial t}|_{shrinkage} = \frac{1}{V}\frac{\partial V}{\partial t} = -\frac{1}{\rho}\frac{\partial \rho}{\partial t}$$
(2.5)

where V is the volume a control volume, and ρ is the density of the liquid alloy. The volumetric liquid feeding rate is calculated by Darcy's Law.

Niyama's model does not account for the solidification of the alloy, while Feurer's model does not account for the mechanical deformation of the mushy region.

2.2.4 RDG Hot Tear Criterion

Recently, Rappaz, Drezet and Gremaud published their mechanistically-based hot tearing criterion, which is one of the liquid feeding criteria [87] called the RDG criterion.
The RDG criterion integrates Darcy's equation over the mushy region to obtain the liquid pressure drop in the interdendritic liquid over the liquid feeding region of the mushy region.

$$\Delta p = \frac{180}{\lambda_2^2} \frac{(1+\beta)\mu}{G} \int_{T_S}^{T_L} \frac{E(T)f_s^2}{(1-f_s)^3} dT + \frac{180}{\lambda_2^2} \frac{v_T \beta \mu}{G} \int_{T_S}^{T_L} \frac{f_s^2}{(1-f_s)^2} dT$$
where
$$E(T) = \frac{1}{G} \int f_s \dot{\epsilon}_p dT$$

$$\beta = \frac{\rho_s}{\rho_l} - 1$$
(2.6)

where G is the temperature gradient over the mushy zone, v_T is the moving velocity of the solidification front, f_s is the fraction of solid, $1 + \beta$ is the ratio between solid and liquid density, μ is the viscosity of liquid steel, and λ_2 is the secondary arm spacing. Equation 2.6 establishes the relation between the pressure drop of the interdendritic liquid and the mechanical strain rate over the mushy zone as well as the solidification. The first term on the right hand side of Equation 2.6 represents the liquid pressure drop caused by mechanical deformation, and the second term represents the liquid pressure drop caused by solidification.

If the mechanical strain rate, $\dot{\epsilon}_p$, is assumed constant over the mushy zone, the mechanical strain rate as a function of the liquid pressure drop is obtained by rearranging Equation 2.6.

$$\dot{\epsilon}_{p} = \frac{\Delta p - \frac{180}{\lambda_{2}^{2}} \frac{v_{T} \beta \mu}{G} \int_{T_{S}}^{T_{L}} \frac{f_{s}^{2}}{(1-f_{s})^{2}} dT}{\frac{180}{\lambda_{2}^{2}} \frac{(1+\beta)\mu}{G} \int_{T_{S}}^{T_{L}} (\frac{1}{G} \int f_{s} dT) \frac{f_{s}^{2}}{(1-f_{s})^{3}} dT}$$
(2.7)

Either liquid pressure or the mechanical deformation strain rate can be used to compare to its critical value to determine the initiation of hot tearing cracks. The RDG criterion assumes hot tear cracks initiate when gas bubbles nucleate. It is addressed as: hot tear cracks initiate when [116]

$$\Delta p \ge p_{cap} + \rho_l gh \tag{2.8}$$

where p_{cap} is the capillary pressure. RDG criterion can be expressed in another form as: hot tear cracks initiate when

$$\dot{\epsilon}_p \ge \dot{\epsilon}_{crit} \tag{2.9}$$

where $\dot{\epsilon}_{crit}$ is calculated using Equation 2.7 by substituting $\Delta p = p_{cap} + \rho_l gh$.

Equations 2.6 or 2.7 acts as a simplified interdendritic flow model to get liquid pressure from the mechanical strain rate of the mushy zone because there is lack of mechanical model to predict interdendritic liquid pressure. The drawback of this approach is that it loses the interaction between the interdendritic liquid flow and the mechanical deformation. At the same time, a reasonable mushy zone mechanical model is still needed to get a good strain rate. Therefore, using RDG model without a good mushy zone mechanical model is lack of eligibility.

Moreover, RDG model made some simplifications which are too important to neglect in author's opinion. Firstly, only solidification shrinkage is considered in RDG model, the thermal shrinkage of liquid and solid phases are both neglected. This might have great effect to the hot tearing crack initiation especially when the solid fraction is close to 1. Secondly, the permeability model only considered the effects of the fraction of solid and the secondary arm spacing. Permeability experiments showed that both the primary and secondary dendrite arm spacings will affect the interdendritic flow [117]. The primary dendrite arm spacing cannot be neglected especially for the flow parallel to the primary dendrite arms. In addition, grain size also affects the permeability because hot tear cracks are always found at the grain boundaries.

Both mechanical and permeability models of the mushy zone are needed to use the RDG hot tearing criterion, Equation 2.8 and 2.9. However, neither of them is available for casting steels due to lack of experimental data. As a consequence, the strain criterion backed by critical strain measurements, described in Section 2.2.2, is chosen to predict hot tear cracks in this work. A mechanical model of mushy zone is initiated in next chapter as a first step to use more comprehensive hot tear criteria such as the RDG model.

2.3 Constitutive Models of Mushy and Liquid Steels

Steels in the mushy and liquid regions behave differently than in their solid state. A proper constitutive model for mushy and liquid steels is very important for a stress model dealing with materials under solidification especially when the interest is near the solidification front such as to predict hot tear cracks.

2.3.1 Treatment of Liquid Steel

Liquid can undergo large shear deformation without generating large stresses. For a classical Newtonian fluid which liquid steel is always considered to be, the shear stress tensor is proportional to its velocity gradient.

$$\boldsymbol{\tau} = \boldsymbol{\mu} (\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^T) = 2\boldsymbol{\mu} \dot{\boldsymbol{\epsilon}'}$$
(2.10)

where μ is the dynamic viscosity of the liquid steel. The strain rate in a typical steel continuous casting process is much less than $0.1sec^{-1}$ [58]. The viscosity of the liquid steel is $0.056Pa \cdot sec^{-1}$ [118]. Thus, the shear stress in the liquid is less than 0.01Pa. This is over 8 orders of magnitude smaller than the stress in the solid on the order of MPa. Therefore, variations in the stress state in the liquid will not affect the stress state in the solid.

One way to treat the liquid is just to take the liquid out of the system based on the above argument. Some models do not assemble the liquid elements into the stiffness matrix [44,51, 119], and apply the hydrostatic pressure directly onto the solid/liquid interface. This method is easy for steady state casting models where the solidification front is stationary. When the solidification front moves with time, this method involves another numerical challenge, the adaptive meshing technique [120].

An alternative way to deal with the liquid elements in transient models [24, 31, 32, 35, 38, 41, 48] is to use a fixed mesh and apply appropriate constitutive models for mechanical behavior of those liquid elements based on the temperature field. This avoids adaptive

meshing. However, a robust numerical integrating technique is needed to integrate two very different constitutive models, solid and liquid, over one domain. It is also common to apply an artificial low value of elastic modulus to those liquid elements to avoid integrating two different constitutive models [19,20,35,36]. This is acceptable for the models only interested in the stress in solid, but not for the models that need realistic stress/strain distribution such as those recent works [48,53,121] that try to predict hot tear cracks in the mushy zone.

2.3.2 Mechanical Behavior of Material in the Mushy State

As research interests turn to how hot tear cracks initiate and propagate, a realistic constitutive model of the partially solidified metal is needed to get the stress/strain distribution within the mushy region because hot tear cracks initiate in the nearly solidified mushy region due to a lack of liquid feeding [114]. Another motivation is that it will benefit the mushy state metal working industry which processes materials in the temperature range that both solid and liquid exist [122].

Gunasekera's Model

Many pioneer researchers in as early as late 1960's and early 1970's conducted the study of the mechanical strength of the semi-solid aluminum alloys with equiaxed structure by tensile test [96] and compression test [123, 124], and the rheology behavior of the lead alloys by compression test [125] and shear test [126, 127]. Their results revealed that the macroscopic deformation of the mushy state materials is dominated by the amount of liquid component because the liquid makes the solid grains easily slip, deform, and rotate when the overall deformation is within 5% [123]. The shear test indicated that in the mushy region, the partially solidified metals are not Newtonian fluids anymore. The viscosity of the mush increases dramatically as the volume fraction of the liquid drops. The mushy viscosity is less than one order of magnitude lower than that of the solid when the volume fraction of the liquid is below 40%. Since then, the mechanical behavior of the mushy state materials has been receiving increasing attentions [128–132] in aluminum industry.

Based on these observations, Gunasekera proposed a theoretical constitutive model of metals in the mushy state following the classical J2 plasticity theory used in solid state materials [122]. This model has the following form:

$$\sigma_{mushy} = \delta \sigma_{solid}$$
where
$$\delta = 1 - (\beta f_l)^{2/3}$$
(2.11)

where σ_{mushy} and σ_{solid} are the stresses over a control volume with mush and solid, respectively. Stress in the solid can take a traditional solid constitutive model. f_l is the volume fraction of the liquid, and β is a constant that depends on the geometric model chosen. Gunasekera calculated the value of β for different geometries of the solid and liquid components in the mushy region, and compared the results to experimental measurements of mushy state metal flow stress. This model, although works well for semi-solid metal forming applications [133, 134], only predicts the overall behavior of the mushy region. It is limited for prediction of hot tear cracks because some hot tear crack criteria require information on the interdendritic liquid pressure, which the Gunasekera model could not predict.

Several experimental works studying the mechanical behavior of steels in mushy state have been published recently. Tseng *et. al.* [113] conducted compression tests in high carbon steels (Carbon content from 0.95 - 1.10%), and fitted the results to the following relationship between the flow stress and the material and the solid fraction:

$$\sigma_f = A e^{B f_s} \tag{2.12}$$

where σ_f and f_s are the flow stress and the solid fraction, respectively. A and B are correlation constants. When the strain of the mushy zone is below 4%, the values of A and B are 0.6062 and 2.235, respectively. As the strain of mushy zone increases, the value of A decreases, while the value of B increases. This indicates that significance of the fraction of solid increases as the deformation of mushy zone increasing.

Seol et. al. [112], Shin et. al. [111] and Mizukami et. al. [110] conducted tensile tests to measure the tensile strength of the carbon steels in mushy state and the Zero Ductility Temperature (ZDT) as well as the Zero Strength Temperature (ZST). Their results showed that steels in the mushy state fail in a brittle manner due to the liquid film existing between the dendrites and the grain boundaries. The ZDT is very close to the solidus temperature. They also observed that the strength of the mushy state steels depends on the fraction liquid until above ZST where the steels lose all of their strength. The ZST is reported at the temperatures where the solid fraction between 60% and 80%.

These tensile strength measurements of steels in the mushy state make the overall mushy region constitutive model applicable to predict hot tear cracks when critical stress or strain based hot tear criterion is used. Some models [48, 53, 63, 135, 136] included a mushy state constitutive model based on the work of Lee and Kim on the plastic behavior of porous metals [137] which is similar to Gunasekera's model. However, the ratio of the flow stresses between the solid and mushy states is in a different form as follows:

$$\delta = \frac{f_s - f_s^c}{1 - f_s^c} \quad ZDT < T < ZST$$

$$\delta = 0 \qquad ZST < T$$
(2.13)

where δ has the same meaning in Equation 2.11, and f_s and f_s^c are the current fraction of solid at ZST, respectively.

Two-Phase Models Based on Liquid Feeding

A new approach, modeling mushy material by a volume averaged two-phase model [138], has emerged in the last couple of years. These models [128,139–143] solve the two sets of coupled momentum conservation equations and the interdendritic flow equation (Darcy's Law), as well as the mass conservation equation at the same time to predict both the stresses/strains in the solid skeleton and the pressure drop and the velocity field of the interdendritic liquid. The overall behavior of the mushy region is given by the volume average of its components as:

$$\boldsymbol{\sigma}_{mushy} = f_s \boldsymbol{\sigma}_s - f_l p \boldsymbol{I} \tag{2.14}$$

where the subscript s, l, and mushy represent the solid, liquid and mushy region, respectively. I is the identity tensor having the same order as the stress tensor. The addition stress tensor of liquid [144], τ_l , is always neglected based on the low Reynold's number of the Newtonian flow through dendrite structures.

This model, although under development, has great potential for broader applications, especially for predicting hot tear cracks, because it covers both of the hot tear criteria, based on thermal induced deformation mechanism and liquid feeding mechanism as discussed in the previous section.

2.4 Figures and Tables



Fig. 2.1: Sequence showing nucleation of a hot tear as two pores in an initially healed hot tear [3]



Fig. 2.2: SEM image with close-ups of a torn-apart solidified bridge on a hot tear surface in an Al-3wt.% Cu alloy showing a deformed surface structure on the main part of the spike and an undeformed draped-looking shape near the root [3]

Chapter 3. Modeling of Semi-Solid Steel

3.1 Governing Equations in Mushy Region

3.1.1 Density Constitutive Equations

Density is a function of temperature, T, and pressure, p, according to the theory of thermodynamics [144]. Consider a material volume V (Figure 3.1) with original dimensions dx_0 , dy_0 , and dz_0 along the three axes x, y, and z, respectively. Assuming mass is conserved within V, then the following expression is true according to mass conservation.

$$\dot{m} = \frac{D(\rho V)}{Dt} = 0 \tag{3.1}$$

$$\rho_0 V_0 = \rho V \tag{3.2}$$

where ρ_0 and V_0 are the density and the volume at an arbitrary chosen state, T_0 , and p_0 . Once the material volume deforms from its original shape because of a change in temperature or pressure or both, the lengths of its three dimensions change as a function of its true strain, $\epsilon = ln \frac{l}{l_0}$, as follows.

$$dx = dx_0 e^{\epsilon_x}$$

$$dy = dy_0 e^{\epsilon_y}$$

$$dz = dz_0 e^{\epsilon_z}$$
(3.3)

where ϵ_x , ϵ_y and ϵ_z are the strain components along axes x, y, and z. It is assumed that the liquid elements do have rigid rotation. This is valid in CON2D where the liquid turbulence is neglected.

Taking the material volume as

$$V_0 = dx_0 dy_0 dz_0 \tag{3.4}$$
$$V = dx dy dz$$

Substituting Equations 3.3 and 3.4 into Equation 3.2 yields

$$\rho = \rho_0 e^{-tr(\boldsymbol{\epsilon})} \tag{3.5}$$

where $tr(\boldsymbol{\epsilon})$ is the trace of the infinitesimal strain tensor, $\boldsymbol{\epsilon}$, which is defined as

$$\boldsymbol{\epsilon} = \frac{1}{2} (\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^T) \tag{3.6}$$

Thus, the time derivative of density can be expressed as

$$\frac{D\rho}{Dt} = -\rho_0 e^{-tr(\boldsymbol{\epsilon})} tr(\dot{\boldsymbol{\epsilon}}) = -\rho tr(\dot{\boldsymbol{\epsilon}})$$
(3.7)

where $\dot{\boldsymbol{\epsilon}}$ is the total strain rate tensor, which is defined as

$$\dot{\boldsymbol{\epsilon}} = \frac{1}{2} (\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^T) \tag{3.8}$$

3.1.2 Conservation of Mass and Momentum

Mass Conservation of Single Phase Solid

The principal of mass conservation states: mass is neither created or consumed [144]. Applying the chain rule to Equation 3.1, it can be rewritten over an arbitrary material volume, V(t), as:

$$\frac{DM}{Dt} = \frac{D\rho}{Dt}V + \rho\frac{DV}{Dt} = 0$$
(3.9)

where M is the total mass in the material volume, V(t). Dividing the volume, V, from the right hand side of Equation 3.9 generates

$$\frac{D\rho}{Dt} + \rho \frac{1}{V} \frac{DV}{Dt} = 0 \tag{3.10}$$

Considering an arbitrary volume, the second term on the LHS of Equation 3.10 can be rewritten as the following, based on definition of strain rate [145].

$$\frac{1}{V}\frac{dV}{dt} = tr(\dot{\boldsymbol{\epsilon}}) \tag{3.11}$$

$$\frac{1}{V}\frac{dV}{dt} = \nabla \cdot \boldsymbol{v} \tag{3.12}$$

where \boldsymbol{v} is the velocity vector of the material points. Equations 3.11 and 3.12 are the volumetric deformation rate, respectively. When the material points have non-zero velocity with respect to their frame of reference, $\frac{D}{Dt}$ is the material derivative operator

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \boldsymbol{v} \cdot \nabla \tag{3.13}$$

Combining Equations 3.10, 3.12 and 3.13 together, the classical mass conservation equation (Equation 3.1) can be written as [144]

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = 0 \tag{3.14}$$

To better understand the physical meaning of Equation 3.14, integrating it over an arbitrary volume, V, gives

$$\int_{V} \frac{\partial \rho}{\partial t} dV = -\int_{V} \nabla \cdot (\rho \boldsymbol{v}) dV$$
(3.15)

Applying the divergence theorem, the RHS of Equation 3.15 becomes the surface integral over the boundary of the volume, V

$$\int_{V} \frac{\partial \rho}{\partial t} dV = -\int_{A} \rho \boldsymbol{v} \cdot \hat{\boldsymbol{n}} dA$$
(3.16)

where $\hat{\boldsymbol{n}}$ is the normal vector of the surface A. Equation 3.16 shows that mass flow across the volume boundary, A, is needed to compensate the density change due to thermal shrinkage/expansion or mechanical deformation [144]. Substituting Equations 3.7 and 3.11 into Equation 3.14 leads to

$$-tr(\dot{\boldsymbol{\epsilon}}) + tr(\dot{\boldsymbol{\epsilon}}) = 0 \tag{3.17}$$

This trivial equation indicates the mass conservation is automatically taken care of in solid mechanics, so long as Equations 3.7 and 3.11 are satisfied.

Mass Conservation of Single Phase Liquid

Equation 3.14 is applicable to any single-phase domain including either solid or liquid. Classic solid mechanics approach does not require explicit satisfaction of it as Equations 3.7 and 3.11 are always satisfied. However, in fluid dynamics, the mass conservation equation has to be explicitly included in the governing equations. This requires Equation 3.14 to be solved for problems such as continuous casting, where the liquid metal is in an open space, and is generally free to flow into and out of the computational domain.

Two Phase Region Mass Conservation

A formal analysis of the mushy region using spacial averaging technique over an arbitrary material volume containing both solid and liquid (Figure 3.2) yields the following equations for mass conservation [138]:

$$\frac{\partial (f_s \rho_s)}{\partial t} + \nabla \cdot (f_s \rho_s \boldsymbol{v}_s) = \Gamma_s \tag{3.18}$$

$$\frac{\partial (f_l \rho_l)}{\partial t} + \nabla \cdot (f_l \rho_l \boldsymbol{v}_l) = -\Gamma_s \tag{3.19}$$

where f_l , f_s , ρ_l , ρ_s , \boldsymbol{v}_l , and \boldsymbol{v}_s are the volume fractions, densities, and velocity vectors of liquid and solid spacial averaged over V in Figure 3.2, and Γ is the specific mass flux $(Kgm^{-3}s^{-1})$ across the internal solid/liquid interface δS in Figure 3.2 due to phase transformation. By assuming that there is no pore or crack formation in the mushy zone, the relation between the fraction of solid and liquid phase is:

$$f_s + f_l = 1$$
 (3.20)

Combining Equations 3.18 and 3.19 together gives

$$\frac{\partial \langle \rho \rangle}{\partial t} + \nabla \cdot (f_s \rho_s \boldsymbol{v}_s) + \nabla \cdot (f_l \rho_l \boldsymbol{v}_l) = 0$$
(3.21)

where $< \rho >$ is defined to be the spacial averaged density of the two phase region as

$$<\rho>=f_s\rho_s+f_l\rho_l\tag{3.22}$$

Adding $\nabla \cdot (f_l \rho_l \boldsymbol{v}_s)$ to both sides of Equation 3.21 and combining terms leads to

$$\frac{D < \rho >}{Dt} + < \rho > \nabla \cdot \boldsymbol{v}_s + \gamma_V = 0 \tag{3.23}$$

where $\gamma_V = \nabla \cdot [f_l \rho_l (\boldsymbol{v}_l - \boldsymbol{v}_s)]$. Note that the first two terms of Equation 3.23 are analogous to the single phase mass conservation, Equation 3.14, if the mushy region is considered as a single material in an averaged manner. An argument left is whether \boldsymbol{v}_s can represent the average velocity of the whole mushy region. This is a reasonable approximation for columnar structures or for an equiaxed structure below the coherency temperature, where a solid skeleton exists. The last term, γ_V , in Equation 3.23 incorporates the phenomenon of interdendritic fluid flow across the material volume boundary δV in Figure 3.2.

3.1.3 Momentum Balance

The momentum balance can then be expressed by [140]:

$$\bar{p}_k \nabla f_k + \nabla \cdot (f_k \boldsymbol{\sigma}_k) + \boldsymbol{M}_k + f_k \rho_k \boldsymbol{g} = \boldsymbol{0}$$
(3.24)

where σ_k is the Cauchy stress tensor of liquid and solid phases, M_k $(Kgm^{-2}s^{-2})$ is the momentum transferred between the liquid and solid phases due to interdendritic fluid drag, g is the acceleration vector of gravity, \bar{p}_k is the average pressure at the solid and liquid interface. k represents either solid, s, or liquid, l. The momentum due to velocity gradients is neglected. In the liquid, this is due to the slow fluid flow, in the mushy zone which is of most interest. In the solid, this is due to the slow velocity under thermal deformation.

The stress tensor of phase k can be decomposed into the deviatoric stress tensor, σ' , and pressure, p_k , as follow:

$$\boldsymbol{\sigma}_{k} = \boldsymbol{\sigma}_{k}^{'} - p_{k}\boldsymbol{I} \tag{3.25}$$

where \boldsymbol{I} is the identity tensor.

The average pressure at the solid and liquid interface δS , \bar{p}_k , equals to the liquid pressure in the material volume, p_l , due to the local instantaneous pressure equilibrium. The momentum balance equations for the solid and liquid phases (Equation 3.24) then can be simplified as:

$$p_l \nabla f_s + \nabla \cdot (f_s \boldsymbol{\sigma}_s) + \boldsymbol{M} + f_s \rho_s \boldsymbol{g} = \boldsymbol{0}$$
(3.26)

$$p_l \nabla f_l + \nabla \cdot (f_l \boldsymbol{\sigma}_l) - \boldsymbol{M} + f_l \rho_l \boldsymbol{g} = \boldsymbol{0}$$
(3.27)

Adding Equations 3.26 and 3.27 leads to the momentum governing equation for the mushy region:

$$\nabla \cdot (f_s \boldsymbol{\sigma}_s + f_l \boldsymbol{\sigma}_l) + (f_s \rho_s + f_l \rho_l) \boldsymbol{g} = \boldsymbol{0}$$
(3.28)

Substituting Equation 3.22 into Equation 3.28 and defining a phase averaged stress, $<\sigma>,$

$$\langle \boldsymbol{\sigma} \rangle = f_s \boldsymbol{\sigma}_s + f_l \boldsymbol{\sigma}_l$$
 (3.29)

similar to the volume average stress of particulate composite materials leads to

$$\nabla \cdot < \boldsymbol{\sigma} > + < \rho > \boldsymbol{g} = \boldsymbol{0} \tag{3.30}$$

This momentum balance equation is the same as the momentum balance equation in classic solid mechanics if the two-phase mushy region is considered as a single phase material in a spatial averaged manner.

3.2 Constitutive Model in Mushy Region

3.2.1 Elastic Constitutive Model

It is assumed that the mushy steel follows the generalized Hook's law as if it was single phase solid steel.

$$\boldsymbol{\sigma} = \boldsymbol{C} : \boldsymbol{\epsilon}^e \tag{3.31}$$

where the stress tensor, $\boldsymbol{\sigma}$, and elastic strain tensor, $\boldsymbol{\epsilon}^{e}$, are the spacial average values as defined in the previous section. \boldsymbol{C} is the fourth order tensor containing the elastic constants. The elasticity tensor \boldsymbol{C} contains only two independent components by assuming the steel in the mushy region to be isotropic. Then, the isotropic linear elastic stress-strain relation in indicial notation is

$$\sigma_{ij} = \lambda \delta_{ij} \epsilon^e_{kk} + 2\mu \epsilon^e_{ij} \tag{3.32}$$

where λ and μ are known as Lame constants. In particular, $\mu = G$, the shear modulus. If we choose Young's modulus and Poisson's ratio as the two elastic constants, the Lame constants are

$$\lambda = \frac{\nu E}{(1+\nu)(1-2\nu)}$$
(3.33)

$$\mu = \frac{E}{2(1+\nu)} \tag{3.34}$$

Taking the trace on both sides of Equation 3.32 leads to volumetric constitutive relation

$$\sigma_{kk} = 3K\epsilon^e_{kk} \tag{3.35}$$

where $K = \lambda + \frac{2\mu}{3}$ is the bulk modulus. It may also define the deviatoric constitutive relation by taking the deviatoric part of Equation 3.32

$$\sigma'_{ij} = 2\mu\epsilon'^e_{ij} \tag{3.36}$$

where σ'_{ij} and ϵ'^e_{ij} are the deviatoric stress tensor and elastic strain tensor.

3.2.2 Inelastic Constitutive Model

The mass conservation, Equation 3.23, momentum balance, Equation 3.30, and Darcy's Law, Equation 2.2, need to be solved together to predict the mechanical response for a given temperature distribution [143,146]. This is too complex and computationally expensive to be feasible for continuous casting problems. Instead, the interdendritic flow can be considered as a kind of viscoplastic strain because they have the same features:

- It is a permanent deformation because it cannot be recovered once the external load is taken off.
- It is time dependent.

Modeling the mushy zone deformation in this way incorporates the interdendritic flow in a solid mechanics manner without solving fluid flow equations. However, a constitutive model of the mushy region material is needed to define the viscoplastic relation between the stress and strain in the mushy zone.

The microstructure of a solidifying material influences its behavior under thermal or mechanical loading. For an equiaxed structure, such as often encountered during aluminum DC casting and semi-solid processing, its mechanical behavior depends greatly on the volume fraction of the solid as indicated by the experiments of metals in semi-solid state [109– 113]. Semi-solid metals with equiaxed structures behave as liquid at low solid fraction state ($f_s < 40\%$). Solid grains and particles suspended in the liquid metal increase the viscosity of the semi-solid material [126, 127]. The stress in the solid grains approximately equals the hydrostatic pressure of the liquid as they are surrounded by the liquid without much interaction among the solid grains. Therefore, metals in the low solid fraction mushy region can be modelled as a non-Newtonian fluid. As the solid fraction increases above 40% to 60%, the adjacent solid grains begin to connect with each other and form a solid skeleton saturated with liquid metal. Stress could be transmitted through the solid skeleton, and strength begins to build up as the solid fraction increases [109–113]. For a columnar structure, however, which is often encountered during continuous casting of steel, the solid skeleton exists even if the solid fraction is fairly small as the dendrites always connect to the fully solidified metal.

Some constitutive models have been proposed to simulate the behavior of the mushy region with high solid fraction ($f_s > 60\%$) for equiaxed structures [132,143,147,148]. Farup *et. al.* simply used the single solid phase constitutive equation to model the mushy region at high solid fraction by assuming the contribution to the stress state from the liquid is negligible [132]. However, the liquid can have great effect on the stress state of the whole mushy region when the fraction of solid is close to 100% because:

- 1. Driving liquid into and out of a high solid fraction mushy region introduces extra resistance to the external force in addition to the resistance deforming the solid skeleton.
- 2. Liquid which is totally surrounded by a continuous skeleton can take compression and tensile external loads without gas bubble nucleation.

Moreover, liquid pressure is also an important parameter to predict porosity formation which makes it beneficial to include liquid in the mushy zone. Another way to model the mushy region is to treat it as a porous material saturated with liquid. Martin *et. al.* [89, 143, 147, 148] proposed a constitutive model for porous metallic materials saturated with liquid based on the models for dry porous materials [149, 150]. These methods should also be applicable to the columnar structures. A similar method is adopted in this work to develop the constitutive model of the mushy zone and extend to liquid model.

Flow Rule in the Mushy Zone

The mechanical behavior of metals in the semi-solid state is assumed to follow a "unified" viscoplastic flow law [20] in an isotropic manner. This "unified" viscoplastic model assumes viscoplastic flow appear at any stress state. There is no yield criterion explicitly defined in this model. Yield surface can be represented by the flow surface when the strain rate is sufficiently slow $(10^{-5}sec.^{-1})$. The difference in behavior between semi-solid metals and single phase solid metals is that the viscoplastic dissipation is not only a function of the second invariant of their stress tensor (Von Mises stress), but also a function of the first invariant of the stress tensor $(tr(\boldsymbol{\sigma}))$. The dependence of the first invariant of the stress tensor comes from the thermal and mechanical induced deformation of the interdendritic liquid and interdendritic fluid flow described by Darcy's Law. The mechanical pressure, p, and the von Mises stress, σ_{vm} , are defined in solid mechanics manner (positive pressure being tensile) which is opposite to Equation 3.25 in fluid dynamics manner (positive pressure being compression).

$$p = \frac{1}{3}tr(\boldsymbol{\sigma}) \tag{3.37}$$

$$\sigma_{vm} = \left(\frac{3}{2}\boldsymbol{\sigma}':\boldsymbol{\sigma}'\right)^{\frac{1}{2}} \tag{3.38}$$

where σ' is the deviatoric stress tensor defined as

$$\boldsymbol{\sigma}' = \boldsymbol{\sigma} - \frac{1}{3} tr(\boldsymbol{\sigma}) \boldsymbol{I}$$
(3.39)

The viscoplastic dissipation energy also depends on the fraction of solid, f_s . The stress tensor here is the phase-averaged stress in Equation 3.29 over the control volume V in Figure 3.2.

The constitutive model is derived according to classical viscoplastic theory [151]. The viscoplastic potential function, Φ , is assumed to be a function of the mechanical pressure, p, and the von Mises stress, σ_{vm} for an isotropic material. The effect of the third invariant is neglected. The viscoplastic strain rate tensor, $\dot{\boldsymbol{\epsilon}}^{in}$, follows the normality rule

$$\dot{\boldsymbol{\epsilon}}^{in} = \frac{\partial \Phi}{\partial \boldsymbol{\sigma}} \tag{3.40}$$

where

$$\Phi = \Phi(p, \sigma_{vm}) \tag{3.41}$$

where p and σ_{vm} include implicit dependence on phase fractions. Substituting Equation 3.37 into Equation 3.39 and rearranging yield

$$\boldsymbol{\sigma} = p\boldsymbol{I} + \boldsymbol{\sigma}' \tag{3.42}$$

Applying the chain rule to Equation 3.40 leads to

$$\dot{\boldsymbol{\epsilon}}^{in} = \left(\frac{\partial \Phi}{\partial p}\right) \left(\frac{\partial p}{\partial \boldsymbol{\sigma}}\right) + \left(\frac{\partial \Phi}{\partial \sigma_{vm}}\right) \left(\frac{\partial \sigma_{vm}}{\partial \boldsymbol{\sigma}}\right)$$
(3.43)

Substituting Equations 3.37 and 3.38 into Equation 3.43, it can be shown that

$$\dot{\boldsymbol{\epsilon}}^{in} = \left(\frac{\partial \Phi}{\partial p}\right) \left(\frac{1}{3}\boldsymbol{I}\right) + \left(\frac{\partial \Phi}{\partial \sigma_{vm}}\right) \left(\frac{3}{2}\frac{\boldsymbol{\sigma}'}{\sigma_{vm}}\right)$$
(3.44)

Several forms of the potential function have been proposed during the last decade. A detailed literature review can be found in reference [147]. The simplest form of the equivalent stress, σ_{eq} , is adopted here,

$$\sigma_{eq} = \left(Ap^2 + B\sigma_{vm}^2\right)^{\frac{1}{2}} \tag{3.45}$$

where A and B are the functions of the solid fraction. From Equations 3.45, 3.37 and 3.38, it can be shown that

$$\frac{\partial \sigma_{eq}}{\partial \boldsymbol{\sigma}} : \boldsymbol{\sigma} = \sigma_{eq} \tag{3.46}$$

The viscoplastic strain rate, $\dot{\epsilon}_{eq}^{in}$, is defined such that its product with the equivalent stress, σ_{eq} , produces the same viscoplastic dissipation energy as the following inner product of strain rate tensor and stress tensor.

$$\dot{\boldsymbol{\epsilon}}^{in}: \boldsymbol{\sigma} = \dot{\boldsymbol{\epsilon}}^{in}_{eq} \boldsymbol{\sigma}_{eq} \tag{3.47}$$

Applying the chain rule to Equation 3.40 yields

$$\dot{\boldsymbol{\epsilon}}^{in} = \frac{\partial \Phi}{\partial \sigma_{eq}} \frac{\partial \sigma_{eq}}{\partial \boldsymbol{\sigma}} \tag{3.48}$$

Combining Equations 3.46 and 3.48 leads to

$$\dot{\boldsymbol{\epsilon}}^{in}: \boldsymbol{\sigma} = \frac{\partial \Phi}{\partial \sigma_{eq}} \sigma_{eq} \tag{3.49}$$

The equivalent strain rate can be found by comparing Equations 3.47 and 3.49

$$\dot{\epsilon}_{eq}^{in} = \frac{\partial \Phi}{\partial \sigma_{eq}} \tag{3.50}$$

Then, from Equations 3.45, 3.48 and 3.50, the viscoplastic strain rate tensor is represented in terms of the equivalent strain rate as

$$\dot{\boldsymbol{\epsilon}}^{in} = \frac{\dot{\epsilon}^{in}_{eq}}{\sigma_{eq}} \left(\frac{1}{3} A p \boldsymbol{I} + \frac{3}{2} B \boldsymbol{\sigma}' \right) \tag{3.51}$$

The equivalent strain rate is found by substituting the trace and the deviatoric parts of Equation 3.51 into Equation 3.45:

$$\dot{\epsilon}_{eq}^{in} = \left(\frac{1}{A}tr(\dot{\boldsymbol{\epsilon}}^{in})^2 + \frac{2}{3}\frac{1}{B}(\dot{\boldsymbol{\epsilon}}^{in'}:\dot{\boldsymbol{\epsilon}}^{in'})\right)^{\frac{1}{2}}$$
(3.52)

where the deviatoric strain rate tensor is also found from

$$\dot{\boldsymbol{\epsilon}}^{in'} = \dot{\boldsymbol{\epsilon}}^{in} - \frac{1}{3} tr(\dot{\boldsymbol{\epsilon}}^{in}) \tag{3.53}$$

Assuming the behavior of metals at elevated temperature follows the power law

$$\dot{\epsilon}_{eq}^{in} = K(T)\sigma_{eq}^n \tag{3.54}$$

where K(T) is the power law constant as a function of temperature, and n is the power coefficient. This leads to the potential function from 3.43 as follows.

$$\Phi = \frac{K(T)}{n+1} \sigma_{eq}^{n+1} \tag{3.55}$$

Equations 3.45, 3.51, and 3.52 establish the relations between the equivalent strain rate and the full 3-D strain rate tensor. This makes the viscoplastic strain tensor to be calculated by numerically integrating a scaler viscoplastic strain rate instead of a strain rate tensor. Note that when the viscoplastic energy does not depend on the mechanical pressure p, then A = 0 in Equation 3.45. If in addition, B = 1, then Equations 3.45, 3.51, and 3.52 become classical Prandtl-Reuss relations.

Interdendritic Fluid Flow

The pressure dependence of the constitutive model of the mushy steel comes from the interdendritic flow due to thermal and mechanical deformation of the solid skeleton for the dendritic structure and equiaxed structure below the coherency temperature. The pressure and velocity of the interdendritic flow is modelled by the liquid momentum balance equation, Equation 3.27, where the drag momentum, M, is modelled by Darcy's Law.

$$\boldsymbol{M} = \mu f_l^2 \boldsymbol{K}^{-1} \cdot (\boldsymbol{v}_l - \boldsymbol{v}_s) \tag{3.56}$$

Substituting Equations 3.25 and 3.56 into Equation 3.27 leads to

$$-f_l \nabla p_l + \nabla \cdot (f_l \boldsymbol{\sigma}_l) - \mu f_l^2 \boldsymbol{K}^{-1} \cdot (\boldsymbol{v}_l - \boldsymbol{v}_s) + f_l \rho_l \boldsymbol{g} = \boldsymbol{0}$$
(3.57)

Assuming the liquid steel as a Newtonian fluid with constant viscosity, the liquid stress tensor is

$$\boldsymbol{\sigma}_{l} = \mu (\nabla \boldsymbol{v}_{l} + \nabla \boldsymbol{v}_{l}^{T}) \tag{3.58}$$

Taking the deviatoric part of both sides of Equation 3.58 yields

$$\boldsymbol{\sigma}_{l}^{'} = \mu (\nabla \boldsymbol{v}_{l} + \nabla \boldsymbol{v}_{l}^{T}) - \frac{2\mu}{3} (\nabla \cdot \boldsymbol{v}_{l}) \boldsymbol{I} = 2\mu \dot{\boldsymbol{\epsilon}}_{fl}^{'}$$
(3.59)

Consider the liquid steel as an incompressible fluid, then

$$\nabla \cdot \boldsymbol{v}_l = 0 \tag{3.60}$$

Substituting Equations 3.59 and 3.60 into Equation 3.57 leads to

$$-f_l \nabla p_l + 2\mu \nabla^2 (f_l \boldsymbol{v}_l) - \mu f_l^2 \boldsymbol{K}^{-1} \cdot (\boldsymbol{v}_l - \boldsymbol{v}_s) + f_l \rho_l \boldsymbol{g} = \boldsymbol{0}$$
(3.61)

where μ is the dynamic viscosity of the liquid steel (0.056*Pas* at 1550°*C* and assumed constant), and K is the permeability tensor that describes the permeability of the mushy zone in 3-D space. Equation 3.61 is a modified Navier-Stokes equation with Darcy's term representing the drag momentum between the solid and the liquid in the mushy zone. The inertia term is neglected which is valid for a low velocity field such as the interdendritic flow.

Equation 3.61 can be simplified into different forms at different locations within the mushy zone: low solid fraction region, coherency region, and the region in between. Details for each of these cases will be presented in Section 3.2.3.

Permeability

Permeability of the mushy region is the key parameter to model the mushy zone mechanical behavior. Its value depends on the microstructure of the mushy zone, equiaxed or columnar, the solid and liquid fractions, the primary and secondary dendrite spacings [117]. Permeability is described by the permeability tensor, \boldsymbol{K} , which is a symmetrical 2nd order tensor. As a stress tensor, all components of the permeability tensor are non-zero in general. However, in a certain frame of reference whose axes of the coordinate system are along the principal flow directions, the off-diagonal components in \boldsymbol{K} vanish. Each main diagonal term represents the permeability along one principal direction.

The permeability of a columnar-dendrite structure is anisotropic due to its directional nature [152–154]. The principal flow directions are parallel and normal to the primary dendrite arms. Therefore, the permeability tensor for columnar structures in a coordinate system with one axis (axis 1 for example) along the primary dendrite arms has non-zero main diagonal components, k_{11} , k_{22} , and k_{33} , only. The dendrite structures in the plane perpendicular to the primary dendrite arms are considered isotropic when the material volume, V, contains enough number of dendrites and the secondary dendrite arms are randomly orientated. As a consequence, $k_{11} \neq k_{22} = k_{33}$. Poirier proposed several empirical equations of the permeability parallel and normal to the primary dendrite arms by fitting several measurements of Pb-Sn systems [117, 152, 155] and borneol-paraffin systems [153, 154]. He indicated that both primary and secondary dendrite arm spacings influence the permeability of the flow normal to the primary dendrite arms, while only primary dendrite arm spacing influences the permeability of the flow parallel to the primary dendrite arms.

A more special case is that all of the main diagonal components of the permeability tensor are equal. This corresponds to a structure with isotropic permeability, such as an equiaxed dendrite structure. For the partially solidified metals with equiaxed dendrite structure such as aluminum, the permeability can be considered isotropic given that enough randomly orientated dendrites are included in the material volume considered. Kozeny-Carman model is always applied for the equiaxed dendrite structures [86].

$$\boldsymbol{K} = \frac{d_2^2}{180} \frac{f_l^3}{(1 - f_l)^2} \boldsymbol{I}$$
(3.62)

where f_l is the fraction of liquid and d_2 is the secondary dendrite arm spacing. This model claims that the primary dendrite arm spacing does not influence the permeability.

3.2.3 Inelastic Constitutive Models for Different Regions in Mushy Zone

Constitutive models are presented here for three regions, low solid fraction region, coherency region, and the region in between. Then, adopting the constitutive model for the isotropic mushy zone (Equations 3.51, 3.52, and 3.53), values for A and B are derived for each region.

Low Solid Fraction Region

In this region the solid fraction is so low that the solid does not influence fluid movement. Therefore, it is reasonable assume the permeability to be infinity $(K \to \infty)$. Following the same argument (solid fraction does not influence liquid movement), the fraction of liquid is assumed to be constant within this region ($\nabla f_l = 0$). As a consequence, Equation 3.61 becomes the Navier-Stokes Equation.

$$-\nabla p_l + 2\mu \nabla^2(\boldsymbol{v}_l) + \rho_l \boldsymbol{g} = \boldsymbol{0}$$
(3.63)

Using Equation 3.59 to replace the second and third terms in Equation 3.63 by the deviatoric liquid stress tensor (σ'_l), Equation 3.63 can be written in the format of solid mechanics as

$$\nabla \cdot \boldsymbol{\sigma}_{l} + \rho_{l} \boldsymbol{g} = \boldsymbol{0} \tag{3.64}$$

where $\boldsymbol{\sigma}_{l} = \boldsymbol{\sigma}_{l}^{'} - p_{l}\boldsymbol{I}$. Using the constitutive model of Newtonian fluid

$$\boldsymbol{\sigma}_l = 2\mu \dot{\boldsymbol{\epsilon}} \tag{3.65}$$

The mushy region with low solid fraction can be considered to be an isotropic material. Then,

$$\sigma_{eq} = 2\mu \dot{\epsilon}_{eq}^{in} \tag{3.66}$$

where σ_{eq} and $\dot{\epsilon}_{eq}^{in}$ are given in Equations 3.45 and 3.52. Comparing Equations 3.65, 3.66, 3.45, 3.51, and 3.52, gives A = 3 and $B = \frac{2}{3}$.

Liquid Impenetrable Region

The solid fraction in this region is so high that the remaining liquid is totally surrounded by solid and isolated from the liquid pool. This is true when the temperature of the mushy region is lower than the coherency temperature and a continuous solid structure forms. Thus, the permeability is zero.

Rearranging Equation 3.61 gives

$$\boldsymbol{v}_{l} - \boldsymbol{v}_{s} = \frac{\boldsymbol{K}}{\mu f_{l}^{2}} \cdot \left[-f_{l} \nabla p_{l} + 2\mu \nabla^{2} (f_{l} \boldsymbol{v}_{l}) + f_{l} \rho_{l} \boldsymbol{g} \right]$$
(3.67)

As the permeability equals to zero, Equation 3.67 yields that

$$\boldsymbol{v}_l - \boldsymbol{v}_s = \boldsymbol{0} \tag{3.68}$$

This implies that when $\mathbf{K} = \mathbf{0}$, the whole mushy region will act as single phase solid, even where the fraction of liquid is not zero yet. Thus, the viscoplastic deformation will follow the solid constitutive model. The solid viscoplastic strain is incompressible which implies $tr(\dot{\boldsymbol{\epsilon}}^{in}) = \mathbf{0}$. Taking trace of both sides of Equation 3.51 immediately determines that A = 0. This indicates that the viscoplastic energy dissipation does not depend on mechanical pressure, but only depends on the deviatoric part of the stress tensor, $\boldsymbol{\sigma}'$. Equations 3.45 and 3.51 then becomes

$$\sigma_{eq} = B^{\frac{1}{2}} \sigma_{vm} \tag{3.69}$$

$$\dot{\boldsymbol{\epsilon}}^{in} = \frac{\dot{\epsilon}_{eq}}{\sigma_{eq}} \frac{3}{2} B \boldsymbol{\sigma}' \tag{3.70}$$

In order to get the value of B in Equations 3.69 and 3.70, an arbitrary material volume V shown in Figure 3.3 is considered under a uniform inelastic strain ϵ^{in} . The stress and strain rate relation is described by the constitutive equation for the solid phase as:

$$\dot{\epsilon}_{vm_s}^{in} = K(T)\sigma_{vm_s}^n \tag{3.71}$$

where $\dot{\epsilon}_{vm_s}^{in}$ and σ_{vm_s} are the von Mises inelastic strain rate and stress of the solid phase material, respectively. Then, the spatially averaged inelastic strain and stress within the material volume V are as follows:

$$\sigma_{eq} = B^{\frac{1}{2}} f_s \sigma_{vm_s} \tag{3.72}$$

$$\dot{\epsilon}_{eq} = \dot{\epsilon}_{vm_s} \tag{3.73}$$

The constitutive equation for the solid phase is adopted for the coherent mushy zone as Equation 3.54. Comparing Equations 3.54, 3.71, 3.72 and 3.73, $B = f_s^{-2}$.

Region Between the Nearly Liquid and Liquid Impenetrable Regions

In this region, liquid flow is limited by the solid skeleton and the liquid pressure is much different than its ferrostatic pressure because of the momentum loss when the liquid flow through this low permeability region. Equations 3.23 and 3.61 need to be solved concurrently to predict the average interdendritic flow velocity and the liquid pressure within the mushy zone. To solve these two equations within the scope of the current solid mechanics, several assumptions are made as follows:

- The reference density, ρ_0 , in Equation 3.7 is chosen to be the liquid density at liquidus, $\rho_l(T_{liquidus})$.
- The deformation of the mushy zone is limited by the solid skeleton, which leads to

$$\boldsymbol{v}_{mushy} = \boldsymbol{v}_s \tag{3.74}$$

where \boldsymbol{v}_{mushy} and \boldsymbol{v}_s are the velocity of the whole mushy zone and the solid skeleton, respectively.

• Mushy zone deformation is small so that the classical small deformation theory is applied here. Moreover, this small deformation assumption implies

$$e^{\epsilon} \approx I$$
 (3.75)

• The momentum due to inertia, diffusion, and shear deformation as well as the effect of gravity of the interdendritic liquid are negligible compared to the Darcy's term in Equation 3.61. The total strain, $\boldsymbol{\epsilon}$, is further decomposed into the sum of the thermal strain, $\boldsymbol{\epsilon}^{th}$, elastic strain, $\boldsymbol{\epsilon}^{e}$, and inelastic strain, $\boldsymbol{\epsilon}^{in}$ as:

$$\boldsymbol{\epsilon} = \boldsymbol{\epsilon}^{th} + \boldsymbol{\epsilon}^{e} + \boldsymbol{\epsilon}^{in} \tag{3.76}$$

$$\boldsymbol{\epsilon}^{in} = \begin{cases} \boldsymbol{\epsilon}^{pl} & \text{in solid} \\ \boldsymbol{\epsilon}^{flow} & \text{in liquid and mush} \end{cases}$$
(3.77)

The first two assumptions as well as Equation 3.7 simplify Equation 3.23 to:

$$\nabla \cdot (f_l(\boldsymbol{v}_l - \boldsymbol{v}_s)) = -tr(\dot{\boldsymbol{\epsilon}}_e + \dot{\boldsymbol{\epsilon}}_{th})e^{tr(\dot{\boldsymbol{\epsilon}}_e + \dot{\boldsymbol{\epsilon}}_{th})} + tr(\dot{\boldsymbol{\epsilon}})e^{tr(\dot{\boldsymbol{\epsilon}})}$$
(3.78)

Define the volumetric flow strain rate as:

$$tr(\dot{\boldsymbol{\epsilon}}_{fl}) = \nabla \cdot (f_l(\boldsymbol{v}_l - \boldsymbol{v}_s)) \tag{3.79}$$

Taking the small strain assumption (Equation 3.75), the mass conservation equation turns to be a strain decomposition equation the same as a classical solid strain decomposition equation as:

$$tr(\dot{\boldsymbol{\epsilon}}) = tr(\dot{\boldsymbol{\epsilon}}_e) + tr(\dot{\boldsymbol{\epsilon}}_{th}) + tr(\dot{\boldsymbol{\epsilon}}_{fl})$$
(3.80)

The last assumption makes Equation 3.61 become Darcy's law:

$$f_l(\boldsymbol{v}_l - \boldsymbol{v}_s) = -\frac{\boldsymbol{K}}{\mu} \cdot \nabla p_l \tag{3.81}$$

Taking ∇ on both sides of Equation 3.81 and using Equation 3.79 to eliminate the velocities give the constitutive equation of the interdendritic liquid.

$$tr(\dot{\boldsymbol{\epsilon}}_{fl}) = -\nabla \cdot \left(\frac{\boldsymbol{K}}{\mu} \cdot \nabla p_l\right)$$
(3.82)

Unlike the classical constitutive equation of the Newtonian fluid, Equation 3.65, the strain rate in Equation 3.82 is a function of pressure gradient. Equation 3.82 is difficult to implement into a solid mechanics model such as CON2D because only displacements are discretized and solved in the modeling domain. The pressure is calculated from the solved displacements for each element. Equation 3.82 cannot be addressed explicitly by this standard displacement formulation. This difficulty may be avoided by using a mixed formulation method in which both displacement and pressure are primary variables at each node [156]. However, the mixed formulation will bring more complexity and stability issues [156].

An approximate method based on the displacement formulation used in CON2D is proposed here. CON2D adopts a parametric 6-node parabolic triangular stress element for the stress model. A parabolic element provides constant pressure gradient, ∇p , within it. Thus, in an element, Equation 3.82 becomes

$$tr(\dot{\boldsymbol{\epsilon}}_{fl}) = -\nabla \cdot \left(\frac{\boldsymbol{K}}{\mu}\right) \cdot \nabla p_l \tag{3.83}$$

For a 2-D system as CON2D, the permeability tensor for columnar dendrite structures is as follows:

$$\boldsymbol{K} = \begin{bmatrix} k_{xx} & k_{xy} \\ k_{yx} & k_{yy} \end{bmatrix} = \begin{bmatrix} k_1 & 0 \\ 0 & k_2 \end{bmatrix} \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}$$
(3.84)

where k_1 and k_2 are the permeability parallel and normal to primary dendrite arms, respectively. $\theta(x, y)$ is the angle between the x-axis of the global coordinate system and the direction of primary dendrite arms. The permeability tensor is a function of fraction of liquid which is finally a function of temperature. Thus, each node has its permeability \mathbf{K}_i where i is the node number. Then, the permeability of any point within an element is as follows

$$\boldsymbol{K} = \sum_{i=1}^{6} N_i \boldsymbol{K}_i \tag{3.85}$$

where N_i is the shape function of the 6-node element shown in Equation B.3. The permeability gradient is

$$\nabla \cdot \boldsymbol{K} = \left\{ \begin{array}{c} \sum_{i=1}^{6} \frac{\partial N_i}{\partial x} k_{xxi} + \sum_{i=1}^{6} \frac{\partial N_i}{\partial x} k_{xyi} \\ \sum_{i=1}^{6} \frac{\partial N_i}{\partial y} k_{xyi} + \sum_{i=1}^{6} \frac{\partial N_i}{\partial y} k_{yyi} \end{array} \right\}$$
(3.86)

The constant pressure gradient is calculated by the pressure values at three Gauss points of each element as follows:

$$\nabla p_l = [B] \left\{ \begin{array}{c} tr(\boldsymbol{\sigma}_1) \\ tr(\boldsymbol{\sigma}_2) \\ tr(\boldsymbol{\sigma}_3) \end{array} \right\}$$
(3.87)

where [B] is the B matrix of a triangle formed by three Gauss points and shown in Equation A.2. σ_1 , σ_2 , and σ_3 are the stress tensor of each Gauss point, respectively.

Comparing the trace of Equation 3.82 and Equation 3.51, it can be determined that

$$A = -\frac{\sigma_{eq}}{\dot{\epsilon}_{eq}^{in}p_l} \nabla \cdot \left(\frac{\mathbf{K}}{\mu} \cdot \nabla p_l\right)$$
(3.88)

The value of $B = f_s^{-2}$ following the same argument as described in the previous section. In this region, σ_{eq} and $\dot{\epsilon}_{eq}^{in}$ are given by Equations 3.45 and 3.52.

3.2.4 Discussion

This model assumes the liquid steel to be an incompressible fluid, which means the dilatational viscosity [144] is neglected. Even the liquid is incompressible, the overall mushy material becomes compressible when the parameter, A, discussed previously is nonzero. This compressibility is purely due to the interdendritic fluid flow through the solidifying dendrites. Note that the stress/strain states in the liquid are solved using the solid mechanics approach with the constitutive model (Equations 3.45, 3.51, and 3.52) described earlier in this section. The inelastic constitutive model in the liquid (Equation 3.66) forces the deviatoric stress in the liquid to be close to zero and pressure to be close to the hydrostatic pressure (ρgh) in

the liquid and low solid fraction regions regardless of the strain state within the scope of the continuous casting process. Under this stress level, the volumetric elastic strain is also forced to be very close to zero by choosing an elastic modulus of the liquid steel (10GPa in this work) and the Poisson's ratio the same as that used in the solid (0.3). This elastic modulus is much larger than the other terms in the system and thus reasonably approximates the impressibility of the liquid steel.

The third approach in the intermediate permeability region is the most general model to predict the behavior of the mushy zone. Equations 3.45, 3.51, and 3.52 collapse to classical equations of von Mises stress, strain and Prandtl-Reuss relations, respectively, in the total solid region ($f_s = 100\%$). They also transform to the equations of the second approach in the liquid impenetrable region when the solid fraction is so high that the permeability is zero. In these two cases ($f_s = 100\%$ or A = 0), only the deviatoric part of the viscoplastic strain rate tensor is nonzero. The sum of the main diagonal terms of the viscoplastic strain rate tensor is always zero indicating no volumetric viscoplastic deformation occurring.

As liquid fraction increase, A and B increase, which act as a penalty to drive liquid pressure towards ferrostatic pressure $(p_l \rightarrow \rho gh)$ and pressure gradient towards small values. In regions with very low solid fractions $(\mathbf{K} \rightarrow \infty \text{ and } f_s \rightarrow 0)$, A and B both go to infinity. This is due to the permeability model being inappropriate in pure liquid region. Thus, this model for intermediate permeability regions should be cut off at some small fraction of solid, when A and B have increased toward their values for Newtonian fluid of 3 and $\frac{3}{2}$, respectively. This approach takes into accounts for anisotropy of the mushy zone permeability, but does not include the anisotropy of material strength, which would require consideration of crystal orientation and reformulation of constitutive equations. In addition, grain boundaries should be incorporated into the mushy zone permeability because hot tears usually occur at the grain boundaries in steel casting.

The third approach in the intermediate permeability region including Darcy's term presented previously would allow use of the RDG hot tear criterion. However, lack of permeability measurements in iron-carbon systems limits the usage of this model. Instead, a simplified empirical hot tear criterion developed by Won [21] is adopted in this work. This criterion puts the inelastic strain rate $\dot{\epsilon}^{in}$ and the brittle temperature range ΔT_B into the denominator of the critical strain equation (Equation 2.1). This implies that higher inelastic strain rate and larger brittle temperature range make hot tear cracks initiate more easily. This agrees with the RDG criterion (Equation 2.6) that larger strain rate and wider mushy zone temperature range leads to larger liquid pressure drop, and increasing cracking tendency. Here the brittle temperature range between 90% and 99% of solid can roughly be considered proportional to the mushy zone temperature range which is between 0% and 100% of solid.

The mushy zone adopted by in this work is the constitutive model for the low solid fraction region, where the mushy zone permeability is infinity $(K \to \infty)$. This approach minimizes the resistance the interdendritic flow and, thus, maximizes the deformability of the mushy zone. Combined with the strain hot tear criterion, this approach results in a conservative hot tear prediction.

3.3 Figures and Tables







Fig. 3.2: General material volume in mushy zone with both solid and liquid



Fig. 3.3: Stress and strain within a material volume

Chapter 4. Model Description

A thermal-mechanical finite element model, CON2D, has been developed at the University of Illinois over the past decade [157]. It is able to simulate temperature, stress, and shape development during the continuous casting of steel, both in and below the mold. The stress model features an elastic-viscoplastic creep constitutive equation that accounts for the different responses of the liquid, semi-solid, δ -ferrite, and austenite phases. Temperature and composition-dependent functions are also employed for properties such as thermal linear expansion. A contact algorithm is developed to prevent penetration of the shell into the mold wall due to the internal liquid pressure. An efficient two-step algorithm has been developed to integrate these highly non-linear equations. An inelastic strain damage criterion is implemented to predict hot tear crack formation, which includes the contribution of pseudo-strain due to the flow of the liquid during feeding of the mushy zone. A thermal resistor model over the interfacial layer between the mold wall and the shell surface makes the heat transfer and stress models fully coupled. This allows CON2D to simulate the continuous casting process under realistic conditions. The model is validated with an analytical solution for both temperature and stress in a solidifying plate. It is then applied to simulate a plant trial of a billet casting to extend the validation. CON2D predicted mold temperature and shell thickness are compared to the plant measurements. This chapter describes all the features of CON2D in detail.

4.1 Heat Transfer Model

CON2D solves the transient energy balance, Equation 4.1, in a transverse Lagrangian reference frame moving downward with the steel shell at the casting speed shown in Figure 4.1.

$$\rho \frac{\partial H(T)}{\partial t} = \nabla \cdot (k(T)\nabla T) \tag{4.1}$$
where H(T) and k(T) are isotropic temperature dependent enthalpy and conductivity of the steel. A 2-D simplification of the full 3-D process is reasonable because the axial heat conduction (along the casting direction) is trivial at the high *Péclet* number of the continuous casting process ($vL/\alpha = 2098$).

Applying the chain rule to the left hand side of Equation 4.1 combines the specific heat, c_p , and the latent heat, L_f , in a convenient function, $\partial H/\partial T$, in Equation 4.2.

$$\rho \frac{\partial H(T)}{\partial T} \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(k(T) \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k(T) \frac{\partial T}{\partial y} \right)$$
(4.2)

Heat balance numerical errors are lessened by providing an enthalpy-temperature look-up function.

Boundary conditions can be fixed temperature, heat flux, convection, or a heat resistor model across the interfacial layer between the mold wall and steel surface [144]. The latter enables the fully coupled heat transfer and stress analysis described in Section 4.5. The thermal property functions of steels, including conductivity and enthalpy, are given in Section 4.9.

4.2 Stress Model

4.2.1 Governing Equation

For the static mechanics problem in this Lagrangian frame, the general governing equation is given by the momentum balance in Equation 4.3.

$$\nabla \cdot \boldsymbol{\sigma} + \rho \boldsymbol{b} = \boldsymbol{0} \tag{4.3}$$

Below the meniscus region, axial temperature and the corresponding displacement gradients are generally small, so it is reasonable to apply a generalized plane strain assumption along the casting direction. This enables a 2-D transient stress analysis to provide a reasonable approximation of the complete 3-D stress state. Although this is not quite as accurate as a fully 3-D analysis [54], this moving slice model approach can realistically model the entire continuous casting process, with a possible exception of the meniscus region, at a relatively small computational cost.

The incremental governing equations acting over each time step, Δt , for the generalized plane strain condition, simplifies Equation 4.3 to the following:

$$\frac{\partial \nabla \sigma_x}{\partial x} + \frac{\partial \nabla \tau_{xy}}{\partial y} = 0$$

$$\frac{\partial \nabla \sigma_y}{\partial y} + \frac{\partial \nabla \tau_{xy}}{\partial x} = 0$$

$$\int \Delta \sigma_z dA = \Delta F_z$$

$$\int x \Delta \sigma_z dA = \Delta M_x$$

$$\int y \Delta \sigma_z dA = \Delta M_y$$
(4.4)

Incremental total strains $\{\Delta \epsilon\}$ are related to displacements $\{u_x, u_y, u_z\}$ according to Equation 4.5.

$$\Delta \epsilon_x = \frac{\partial \Delta u_x}{\partial x}$$

$$\Delta \epsilon_y = \frac{\partial \Delta u_y}{\partial y}$$

$$\Delta \epsilon_{xy} = \frac{1}{2} \left(\frac{\partial \Delta u_y}{\partial x} + \frac{\partial \Delta u_x}{\partial y} \right)$$

$$\Delta \epsilon_z = a + bx + cy$$
(4.5)

There are no body forces because the ferrostatic pressure caused by gravity acting on the liquid is instead applied through the internal boundary conditions, as described in Section 4.7. Besides the usual boundary conditions such as fixed displacements and surface tractions, a special type of boundary condition, mold wall constraint, is included in CON2D to model the interactions between the mold wall and the steel surface as addressed in Section 4.6. The shape of the mold influences the temperature and stress of the steel greatly as the interaction between the mold and the shell occurring. This is also discussed in Section 4.6.

Two fold symmetry can be assumed in the current continuous casting applications, so the constants related to bending, b and c in Equation 4.5 and ∇M_x and ∇M_y in Equation 4.4 all vanish and $\Delta \epsilon_z$ represents the unconstraint axial (thickness) contraction of each 2-D slice.

4.2.2 Constitutive Equations

Stress-Strain Relationship

Increments of stress and elastic strain are related through Hook's law, Equation 4.6.

$$\{\Delta\sigma\} = [D]\{\Delta\epsilon_e\} + [\Delta D]\{\epsilon_e\}$$
where,
$$\{\sigma\} = \{ \sigma_x \ \sigma_y \ \sigma_z \ \tau_{xy} \}^T$$

$$\{\epsilon\} = \{ \epsilon_x \ \epsilon_y \ \epsilon_z \ \epsilon_{xy} \}^T$$
(4.6)

Matrix [D] contains the isotropic temperature-dependent elastic modulus, E(T), and Poisson's ratio, ν , given in Equation 4.7.

$$[D] = \frac{E(T)}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1-\nu & \nu & 0 & \nu \\ \nu & 1-\nu & 0 & \nu \\ 0 & 0 & \frac{1-2\nu}{2} & 0 \\ \nu & \nu & 0 & 1-\nu \end{bmatrix}$$
(4.7)

The incremental total strains, $\{\Delta\epsilon\}$, in Equation 4.5 are composed of elastic strain, $\{\Delta\epsilon_e\}$, thermal strain, $\{\Delta\epsilon_{th}\}$, inelastic strain, $\{\Delta\epsilon_{in}\}$, and flow strain, $\{\Delta\epsilon_{fl}\}$, components as given in Equation 4.8.

$$\{\Delta\epsilon\} = \{\Delta\epsilon_e\} + \{\Delta\epsilon_{th}\} + \{\Delta\epsilon_{in}\} + \{\Delta\epsilon_{fl}\}$$
(4.8)

Totals of all strains at a given time, $t+\Delta t$, are obtained by accumulating the strain increments at each prior time step. For example, the total strain is accumulated as follows, Equation 4.9, while the other strains are accumulated similarly.

$$\{\epsilon^{t+\Delta t}\} = \{\epsilon^t\} + \{\Delta\epsilon^{t+\Delta t}\}$$

$$(4.9)$$

Thermal Strain

Thermal strain arises due to volume changes caused by both temperature differences and phase transformations, including solidification and solid-state phase changes between crystal structures, such as austenite and ferrite. The incremental isotropic thermal strain vector, $\{\Delta \epsilon_{th}\}$, given in Equation 4.10, is based on the phase fractions and the thermal linear expansion function, *TLE*, discussed in Section 4.9.

$$\{\Delta \epsilon_{th}\} = (TLE(T^t) - TLE(T^{t-\Delta t}))\{1 \ 1 \ 0 \ 1\}^T$$
(4.10)

Inelastic Strain

Inelastic strain includes both strain-rate independent plasticity and time dependent creep. Creep is significant at the high temperatures during the continuous casting process and is indistinguishable from the plastic strain. Thus, this work adopts a unified constitutive model of the mechanical behavior to capture the temperature- and strain-rate sensitivity of high temperature steel.

The inelastic strain rate, $\dot{\epsilon}_{in}$, is described by different constitutive models according to microstructural state of the solid steel.

$$\dot{\bar{\epsilon}}_{in} = \begin{cases} \dot{\bar{\epsilon}}_{pl-\delta} &, \%\delta \ge 10\%, T \le T_{coherency} \\ \dot{\bar{\epsilon}}_{pl-\gamma} &, \%\delta \le 10\%, T \le T_{coherency} \\ \dot{\bar{\epsilon}}_{flow} &, T > T_{coherency} \end{cases}$$
(4.11)

where $\dot{\epsilon}_{pl-\delta}$ and $\dot{\epsilon}_{pl-\gamma}$ are the equivalent inelastic strain rates of ferrite and austenite, respectively, as given in Section 4.9.4. $\dot{\epsilon}_{flow}$ and $T_{coherency}$ are the equivalent flow strain rate and the coherency temperature defined in the next section. The inelastic strain rate function follows the ferrite function (δ or α) in solid, whenever the phase fraction of ferrite exceeds 10% of the total volume. This is justified by considering the steel with two phases as a composite material in which only a small amount of the weaker ferrite phase weakens the mechanical strength of the whole material.

The plain carbon steels treated in this work are assumed to harden isotropically, so the von Mises loading surface, associated plasticity and normality hypothesis in the Prandtl-Reuss flow law is applied [151]:

$$\dot{\boldsymbol{\epsilon}}_{in} = \frac{3}{2} \dot{\bar{\boldsymbol{\epsilon}}}_{in} \frac{\boldsymbol{\sigma}'}{\bar{\boldsymbol{\sigma}}} \tag{4.12}$$

where $\dot{\boldsymbol{\epsilon}}_{in}$, $\boldsymbol{\sigma}'$, $\bar{\boldsymbol{\sigma}}$ and $\dot{\bar{\boldsymbol{\epsilon}}}_{in}$ are the inelastic strain rate tensor, the deviatoric stress tensor, the equivalent stress scalar and equivalent inelastic strain-rate scalar, respectively. The equivalent strain-rate, $\dot{\bar{\boldsymbol{\epsilon}}}_{in}$, is given as:

$$\dot{\bar{\epsilon}}_{in} = c\sqrt{\frac{2}{3}}\dot{\epsilon}_{in} : \dot{\epsilon}_{in}$$
where
$$c = \begin{cases} \frac{\epsilon_{max}}{|\epsilon_{max}|} & |\epsilon_{max}| \ge |\epsilon_{min}| \\ \frac{\epsilon_{min}}{|\epsilon_{min}|} & |\epsilon_{max}| < |\epsilon_{min}| \end{cases}$$

$$\epsilon_{max} = max(\epsilon_{11}, \epsilon_{22}, \epsilon_{33})$$

$$\epsilon_{min} = min(\epsilon_{11}, \epsilon_{22}, \epsilon_{33})$$
(4.13)

The ":" operator means standard term by term tensor multiplication. In this work, the equivalent inelastic strain rate, $\dot{\epsilon}_{in}$, bears a sign determined by the direction of the maximum principal inelastic strain as defined in Equation 4.13 in order to achieve kinematic behavior (Bauschinger effect) during reverse loading.

Equations 4.12 and 4.13 allows an isotropic scalar to represent the full 3-D strain-rate state. Appendix B defines σ' , $\bar{\sigma}$ and Equation 4.12 in 2-D generalized plane strain form. Parameter c (+1 or -1) makes the equivalent inelastic strain rate have the same sign as the maximum principal inelastic strain. The functions for the inelastic strain rate scalars, $\dot{\bar{\epsilon}}_{in}$, described in Section 4.9, must be integrated to find $\{\Delta \epsilon_{in}\}$ needed in Equation 4.8, as described previously in this section.

Strain in Mushy and Liquid Elements

In this model, the liquid elements are generally given no special treatment regarding material properties and finite element assembly. However, liquid reacts very differently from solid under external loads. It deforms elastically under hydrostatic force as if it was solid but deforms dramatically under shear force. If any liquid is present in a given finite element, a constitutive equation is used to generate an extremely rapid creep rate:

$$\dot{\bar{\epsilon}}_{flow} = \begin{cases} A(|\bar{\sigma}|) & |\bar{\sigma}| > \sigma_{yield} \\ 0 & |\bar{\sigma}| \le \sigma_{yield} \end{cases}$$
(4.14)

The parameter A is chosen to be $1.5 \times 10^8 MPa^{-1} \cdot sec$. to match the viscosity of molten steel [118]. Equation 4.14 is another format of the linear viscous equation [144] of the Newtonian fluid which is a reasonable assumption for the liquid steel in the mushy zone. Liquid deforms under any nonzero shear stress according to Newtonian fluid dynamics. Thus, σ_{yield} should be zero. To avoid numerical difficulty, however, σ_{yield} is treated as a tolerance accuracy parameter without a physical nature and is given a value of 0.01MPa.

This method effectively increases shear strain, and thus enforces negligible liquid strength and shear stress. The critical temperature where the fraction of liquid is sufficient to make the elements act as a liquid is the "coherency temperature", $T_{coherency}$, currently defined equal to the solidus temperature. To generalize this scalar strain-rate to a multi-dimensional strain vector, the same Prandtl-Reuss relations, Equations 4.12 and 4.13, are used as for the solid, $\dot{\epsilon}_{in}$.

This fixed-grid approach avoids the difficulties of adaptive meshing while allowing strain to accumulate in the mushy region. As in the real continuous casting process, the total mass of the liquid domain is not constant. The inelastic strain accumulated in the liquid represents mass transport due to fluid flow, so is denoted "flow strain". Positive flow strain indicates fluid feeding into the region. This is important for the prediction of hot tear cracks. The disadvantage of using this high creep rate function to model liquid is increasing the computational difficulty at the solidification front. This requires the use of a very robust local iteration algorithm [20].

4.3 Finite Element Implementation

4.3.1 Heat Transfer and Solidification Model

The 3-node triangle finite element is employed to approximate temperature distribution in the domain as a piece-wise linear function. The standard Galerkin method [156] applied to Equation 4.2 yields the following global matrix equations.

$$[K] \{T\} + [C] \{\dot{T}\} = \{F_q\} + \{F_{q_{sup}}\}$$
(4.15)

where [K] is the conductance matrix including the effect of conductivity k(T), and [C] is the capacitance matrix including the effect of specific heat, c_p , and latent heat, L_f , in enthalpy, H(T). Within each element, an effective specific heat, c_{pe} , is evaluated using a spatial averaging technique suggested by Lemmon [158].

$$c_{pe} = \frac{\partial H}{\partial T} = \sqrt{\frac{\left(\frac{\partial H}{\partial x}\right)^2 + \left(\frac{\partial H}{\partial y}\right)^2}{\left(\frac{\partial T}{\partial x}\right)^2 + \left(\frac{\partial T}{\partial y}\right)^2}}$$
(4.16)

Enthalpy gradients are interpolated within each element using the standard natural coordinates as shape functions. Average conductivity within each element is obtained by simply averaging the three nodal values. A three-level time-stepping method proposed by Dupont [159] is adopted to solve Equation 4.15. Temperatures at the current time $t + \Delta t$ are found from the temperatures at the previous two time steps, t and $t - \Delta t$.

$$\{T\} = \frac{1}{4} \left\{ 3T^{t+\Delta t} + T^{t-\Delta t} \right\}$$
(4.17)

$$\left\{\dot{T}\right\} = \left\{\frac{T^{t+\Delta t} - T^t}{\Delta t}\right\} \tag{4.18}$$

Substituting Equations 4.17 and 4.18 into Equation 4.15 and rearranging give a recursive global matrix equation expressing the time and spatial discretization of the heat conduction equation, Equation 4.2.

$$\left[\frac{3}{4}\left[K\right] + \frac{[C]}{\Delta t}\right] \left\{T^{t+\Delta t}\right\} = \left\{F_q\right\} + \left\{F_{q_{sup}}\right\} - \frac{1}{4}\left[K\right] \left\{T^{t-\Delta t}\right\} + \frac{[C]}{\Delta t} \left\{T^t\right\}$$
(4.19)

Equation 4.19 is solved at each time step for the unknown nodal temperatures, $T^{t+\Delta t}$, using a Choleski decomposition solver [160]. F_q and $F_{q_{sup}}$ are the heat flow load vectors containing the distributed heat flux at the domain boundary and the super heat flux vector at the internal moving boundary, respectively. On each boundary (between node i and j) where heat flux is applied, the contributions from each element on the boundary are summed as follows:

$$\{F_q\} = \sum_{allboundary elements} \int [N]^T q dL = \sum_{allboundary elements} \begin{cases} \frac{q_{ij}L_{ij}}{2} \\ \frac{q_{ij}L_{ij}}{2} \end{cases}$$
(4.20)

where L_{ij} is the distance between node i and j. The heat flux function, q, will be determined according to specific applications. The super heat flux is applied using the similar method, where the boundary element set and heat flux function are determined differently which are discussed in Section 4.7.1.

4.3.2 Stress Model

Applying the standard Galerkin method to Equations $4.4 \sim 4.7$ gives the set of linear equations over the finite element domain below,

$$[K]\{\Delta u\}^{t+\Delta t} = \{\Delta F_{in}\}^{t+\Delta t} + \{\Delta F_{th}\}^{t+\Delta t} + \{\Delta F_{fp}\}^{t+\Delta t} - \{\Delta F_{el}\}^{t+\Delta t}$$
(4.21)

where [K], $\{\Delta F_{in}\}$, $\{\Delta F_{th}\}$, $\{\Delta F_{fp}\}$, and $\{F_{el}\}$ are the stiffness matrix and incremental force vectors due to incremental thermal strain, inelastic strain, ferrostatic pressure and external surface traction at particular boundaries, and elastic strain corrections from the previous time step, respectively. Refer to Equations B.10 ~ B.14 in Appendix B for more details. At each time step, Equation 4.21 is solved for the incremental displacements, $\{\Delta u\}$, using the Choleski method [160] and the total displacements are updated as

$$\{u\}^{t+\Delta t} = \{u\}^t + \{\Delta u\}$$
(4.22)

Then, the total strains and stresses are updated from Equations 4.5 and 4.6, respectively. The 6-node quadratic-displacement triangle elements use the same grid of nodes that are connected into 3-node elements for the heat flow calculation. Further details are given in Appendix B.

4.4 Numerical Integration Scheme

Highly strain-rate-dependent inelastic models require a robust numerical integration technique to avoid numerical difficulties. The non-linear equations to be integrated are given in Equations 4.23 and 4.24 by combining Equations 4.6 and 4.8, neglecting the second term of the right hand side of Equation 4.8.

$$\boldsymbol{\sigma}^{t+\Delta t} = \boldsymbol{C}^{t+\Delta t} : \left(\boldsymbol{\epsilon}^{t} - \boldsymbol{\epsilon}_{th}^{t} - \boldsymbol{\epsilon}_{in}^{t} + \Delta \boldsymbol{\epsilon}^{t+\Delta t} - \Delta \boldsymbol{\epsilon}_{th}^{t+\Delta t} - \Delta \boldsymbol{\epsilon}_{in}^{t+\Delta t}\right)$$
(4.23)

$$\bar{\epsilon}_{in}^{t+\Delta t} = \bar{\epsilon}_{in}^t + \Delta \bar{\epsilon}_{in}^{t+\Delta t} \tag{4.24}$$

The incremental equivalent inelastic strain accumulated over a time step is given in Equation 4.25 based on a highly nonlinear constitutive function, which depends on $\bar{\sigma}$ and $\bar{\epsilon}_{in}$, which change greatly over the time step.

$$\Delta \bar{\epsilon}_{in}^{t+\Delta t} = F(T, \bar{\sigma}^{t+\Delta t}, \bar{\epsilon}_{in}^{t+\Delta t}, \% C) \Delta t$$
(4.25)

F is one of the constitutive functions given in Equations 4.14, 4.58, or 4.60 depending on the current material state. Substituting Equations 4.12 and 4.25 into Equations 4.23 and 4.24 and using fully implicit time stepping method, a new set of evolution equations are obtained as:

$$\boldsymbol{\sigma}^{t+\Delta t} = \boldsymbol{C}^{t+\Delta t} : \left(\boldsymbol{\epsilon}^{t} - \boldsymbol{\epsilon}_{th}^{t} - \boldsymbol{\epsilon}_{in}^{t} + \Delta \boldsymbol{\epsilon}^{t+\Delta t} - \Delta \boldsymbol{\epsilon}_{th}^{t+\Delta t} - \frac{3}{2} F \frac{\boldsymbol{\sigma}^{t+\Delta t'}}{\bar{\sigma}^{t+\Delta t}} \Delta t\right)$$
(4.26)

$$\bar{\epsilon}_{in}^{t+\Delta t} = \bar{\epsilon}_{in}^t + F(T, \bar{\sigma}^{t+\Delta t}, \bar{\epsilon}_{in}^{t+\Delta t}, \% C) \Delta t$$
(4.27)

Two tensors, $\boldsymbol{\sigma}^{t+\Delta t}$ and $\Delta \boldsymbol{\epsilon}^{t+\Delta t}$, and one scalar, $\bar{\epsilon}_{in}^{t+\Delta t}$, comprise 13 unknown scalar fields for 3-D problems or 9 unknowns for the 2-D problem here, which need solving through Equations 4.26 and 4.27. Zhu implemented an alternating implicit-explicit mixed time integration scheme, which is based on an operator-splitting technique that alternates between local and global forms of the total strain increment and inelastic strain rate over each pair of successive steps [20]. Within each time step, $\boldsymbol{\sigma}^{t+\Delta t}$ and $\bar{\epsilon}_{in}^{t+\Delta t}$ are first solved using a fully implicit time integration technique based on the current best estimation of the total strain increment $\Delta \hat{\boldsymbol{\epsilon}}$, which is taken from the previous time step $\Delta \boldsymbol{\epsilon}^t$. This is a "local step" because it is spatially uncoupled. Then, improved estimates of $\sigma^{t+\Delta t}$ and $\bar{\epsilon}_{in}^{t+\Delta t}$ from the "local step" are used to solve for $\Delta \epsilon^{t+\Delta t}$ by explicit finite element spatial integration through Equations 4.21 and 4.5. This is a "global step" [20]. There is still a tensor unknown in Equation 4.26, which makes even the local time integration step computationally expensive. Lush *et. al.* transformed the tensor equation of Equation 4.26 into a scalar equation for isotropic materials with isotropic hardening [161].

$$\bar{\sigma}^{t+\Delta t} = \bar{\sigma}^{*t+\Delta t} - 3\mu^{t+\Delta t}F(T,\bar{\sigma}^{t+\Delta t},\bar{\epsilon}_{in}^{t+\Delta t},\% C)\Delta t$$
(4.28)

where $\bar{\sigma}^{*t+\Delta t}$ is the equivalent stress of the stress tensor, $\bar{\sigma}^{*t+\Delta t}$, defined below.

$$\boldsymbol{\sigma}^{*t+\Delta t} = \boldsymbol{C}^{t+\Delta t} : (\boldsymbol{\epsilon}^t - \boldsymbol{\epsilon}_{th}^t - \boldsymbol{\epsilon}_{in}^t + \Delta \hat{\boldsymbol{\epsilon}} - \dot{\boldsymbol{\epsilon}}_{th}^{t+\Delta t} \Delta t)$$
(4.29)

Equations 4.27 and 4.28 form a pair of nonlinear scalar equations to solve two unknowns $\bar{\epsilon}_{in}^{t+\Delta t}$ and $\bar{\sigma}^{t+\Delta t}$ by using operator-splitting method within a pair of successive local and global steps. In the local step, a bounded Newton-Raphson iteration scheme [161] is adopted.

The integration procedure used within each time step is summarized as:

- 1. Estimate $\{\Delta \hat{\epsilon}\}$ based on $\{\Delta u\}$ from the previous time step: $\{\Delta \hat{\epsilon}\} = [B] \{\Delta u\}^t$.
- 2. Calculate $\{\sigma^*\}^{t+\Delta t}$, $\hat{\sigma}^*$ and $\{\sigma^{*'}\}^{t+\Delta t}$, needed to define the direction of the stress vector.

$$\{\sigma^*\}^{t+\Delta t} = [D]^{t+\Delta t} \left(\{\epsilon\}^t - \{\epsilon_{th}\}^t - \{\epsilon_{in}\}^{t+\Delta t} + \{\Delta\hat{\epsilon}\} - \dot{\epsilon}_{th}^{t+\Delta t} \Delta t \{1 \ 1 \ 0 \ 1\}^T\right)$$
(4.30)

3. Solve the following two ordinary differential equations simultaneously for $\bar{\epsilon}_{in}^{t+\Delta t}$ and $\bar{\sigma}^{t+\Delta t}$ at each local Gauss point, using a fully implicit bounded Newton-Raphson integration method from Lush [161]. This method gives the best robustness and efficiency of several alternative approaches evaluated [20]. Function F is either Kozlowski model

III for γ , the power law for δ , or flow strain for liquid phase.

$$\bar{\epsilon}_{in}^{t+\Delta t} = \bar{\epsilon}_{in}^{t} + F(T, \bar{\hat{\sigma}}^{t+\Delta t}, \bar{\epsilon}_{in}^{t+\Delta t}, \% C) \Delta t$$

$$\bar{\hat{\sigma}}^{t+\Delta t} = \bar{\sigma}^{*t+\Delta t} - 3\mu^{t+\Delta t} F(T, \bar{\hat{\sigma}}^{t+\Delta t}, \bar{\epsilon}_{in}^{t+\Delta t}, \% C) \Delta t$$
(4.31)

4. Expand this scalar stress estimate into vector form:

$$\{\hat{\sigma}\}^{t+\Delta t} = \bar{\hat{\sigma}}^{t+\Delta t} \frac{\{\sigma^{*'}\}^{t+\Delta t}}{\bar{\sigma}^{*t+\Delta t}} + \frac{1}{3}\sigma_m^{*t+\Delta t}\{\delta\}^T$$

$$\{\sigma^{*'}\}^{t+\Delta t} = \{\sigma^{*}\}^{t+\Delta t} - \frac{1}{3}\sigma_m^{*t+\Delta t}\{\delta\}^T$$

$$\sigma_m^{*t+\Delta t} = \sigma_x^{*t+\Delta t} + \sigma_y^{*t+\Delta t} + \sigma_z^{*t+\Delta t}$$

$$\{\delta\} = \{1 \ 1 \ 0 \ 1 \}$$

$$(4.32)$$

- 5. Calculate $\dot{\epsilon}_{in}^{t+\Delta t}$ from $\bar{\hat{\sigma}}^{t+\Delta t}$ and $\bar{\epsilon}_{in}^{t+\Delta t}$ using F according to the material phase.
- 6. Expand this scalar inelastic strain estimate into a vector $\{\dot{\epsilon}_{in}\}^{t+\Delta t}$ with the same direction as $\{\hat{\sigma}'\}^{t+\Delta t}$ using Prandtl-Reuss relations; Update $\{\epsilon_{in}\}^{t+\Delta t} = \{\epsilon_{in}\}^t + \{\dot{\epsilon}_{in}\}^{t+\Delta t} \Delta t$ only for solidified elements.
- 7. Use classic FEM spatial integration (Appendix B) to solve Equation 4.21 for $\{\Delta u\}^{t+\Delta t}$ based on $\{\dot{\epsilon}_{in}\}^{t+\Delta t}$.
- 8. Finally, find $\{\Delta \epsilon\}^{t+\Delta t}$ from $\{\Delta u\}^{t+\Delta t}$ and update $\{\epsilon\}^{t+\Delta t}$ and $\{\sigma\}^{t+\Delta t}$.

Overall, this alternating implicit-explicit scheme with the bounded Newton-Raphson iteration gives the best robustness and efficiency of several alternative FEM time integration approaches evaluated [20].

4.5 Treatment of the Mold - Shell Interface

Heat transfer does not depend directly on the force equilibrium equation because the mechanical dissipation energy is negligible. The heat flow and stress models are fully coupled

with each other, however, when the gap between mold and steel shell is taken into account. Shrinkage of the shell tends to increase the thermal resistance across the gap where the shell is strong enough to pull away from the mold wall. This leads to hot and weak spots on the shell. This interdependence of the gap size and the thermal resistance requires iteration between the heat transfer and stress models. As the gap size is unknown in prior, the heat resistance is also unknown. Thus, iterations within a time step are usually needed. Contact between the mold wall and shell surface is discussed in Section 4.6.2.

4.5.1 Interface Heat Transfer

When the coupled heat transfer and thermal stress analysis is performed, the heat transfer boundary condition at the steel surface is described by a gap heat resistor model shown in Figure 4.3. Heat leaves the steel shell via conduction and radiation across the interfacial gap. It is then conducted across the thin copper mold, and extracted by cooling water flowing across the back of the mold tube. The temperature and the heat convection coefficient of the cooling water are input from the results of a preliminary computation using the CON1D model, described elsewhere [2]. The contact resistance adopted in this model is several orders of magnitude larger than the physical contact resistance [118] between flat steel and copper surface because it includes the influence of oscillation marks [2]. The gap thickness is calculated during each iteration from the shell surface displacement and the mold wall position, according to the local values of the mold taper and distortion, which are described in the next section. Once the gap size is determined, the heat flux, q_{gap} , across the interfacial layer between the mold wall and steel surface is solved together with the mold hot face temperature, T_{mold} :

$$q_{gap} = -\frac{T_{shell} - T_{water}}{r_{gapmold}}$$
where
$$r_{gapmold} = \frac{1}{h_{water}} + \frac{T_{mold}}{k_{mold}} + \frac{\frac{t_{gap}}{k_{gap}} + r_{contact}}{1 + h_{rad}(\frac{t_{gap}}{k_{gap}} + r_{contact})}$$

$$h_{rad} = \frac{5.67d - 8}{\frac{1}{\varepsilon_m} + \frac{1}{\varepsilon_s} - 1} (T_{shell} + T_{mold}) (T_{shell}^2 + T_{mold}^2)$$

$$\bar{e} = \frac{1}{\frac{1}{\varepsilon_m} + \frac{1}{\varepsilon_s} + 1}$$

$$T_{mold} = \frac{5.67 \times 10^{-8} \bar{e} T_{shell}^4 + \frac{T_{shell}}{r_{mold}} + \frac{T_{water}}{r_{gap}}}{\frac{1}{r_{mold}} + \frac{1}{r_{gap}}}$$

$$r_{mold} = \frac{d_{mold}h_{water} + k_{mold}}{h_{water}k_{mold}}$$

$$r_{gap} = \frac{d_{gap}}{k_{gap}} + r_{contact}$$

$$(4.33)$$

4.5.2 Gap Size Calculation

The gap size, d_{gap} , is calculated online for each boundary node at the shell surface, based on gaps from the previous iteration, n:

$$\hat{d}_{gap}^{n+1} = max(\{u(d_{gap}^{n})\} \cdot \hat{n} - d_{wall}^{t+\Delta t}, d_{gapmin})$$
where
$$d_{wall}^{t+\Delta t} = d_{taper}^{t+\Delta t} - d_{molddist}^{t+\Delta t}$$
(4.34)

where $\{u\}$, \hat{n} , d_{wall} , d_{taper} , $d_{molddist}$ and d_{gapmin} are the displacement vector at boundary nodes, unit normal vector to the mold wall surface, mold wall position, mold wall position change due to mold distortion, and the minimum gap thickness, respectively. A positive d_{gap} , indicates a real space between the mold and shell.

The minimum gap value is set as:

$$d_{gapmin} = r_{contact} k_{gap} \tag{4.35}$$

It physically means the effective oscillation mark depth at the shell surface. When the gap size calculated is less than the minimum gap size, the contact resistance, $r_{contact}$, dominates the heat resistance between the shell surface and the mold wall. Gap size variation within the minimum gap size is assumed not to affect the thermal resistance, which accelerates convergence.

4.5.3 Thermal - Stress Coupling

The overall flow of CON2D is shown in Figure 4.4. Within each time step, the computation alternates between the heat transfer and stress models through the following fullycoupled procedure:

- 1. The temperature field is solved based on the current best estimate of gap size, from the previous time step with Equation 4.34. The initial gap size at the beginning of the simulation is simply zero around the strand perimeter as the liquid steel at the meniscus flows to match the mold contour.
- 2. The incremental thermal strain is evaluated from the temperature field at the current and previous time steps, Equation 4.10. The inelastic strain is estimated by integrating Equation 4.31 following the procedure described in Section 4.4. The global matrix equation, Equation 4.21, is solved for displacements, strains, and stresses using the standard finite element method.
- 3. The gap sizes for the next iteration are updated by:

$$d_{gap}^{n+1} = \beta \hat{d}_{gap}^{n+1} + (1-\beta) d_{gap}^n \tag{4.36}$$

where β is chosen to be 0.5.

4. Finally, steps $1 \sim 3$ are repeated until the gap size difference between two successive heat transfer and stress iterations, n and n + 1, is small enough:

$$d_{diff} = \sqrt{\frac{\sum_{nb} (d_{gap}^{n+1} - d_{gap}^{n})^2}{\sum_{nb} (d_{gap}^{n})^2}}$$
(4.37)

where nb is the number of all boundary nodes. When d_{diff} becomes smaller than the specified "gap tolerance", d_{min} , the gap size is considered converged.

4.6 Modeling the Mold Wall

The mold wall affects the calculation in two ways:

- 1. Altering the size of the interfacial gap and associated heat transfer between the mold and strand through its distorted shape.
- 2. Constraining the shell from bulging due to the internal ferrostatic pressure.

4.6.1 Mold Wall Shape

The mold wall is defined in CON2D as a function of distance below the meniscus. The shape of the mold varies from its dimensions at the meniscus due to mold taper and mold distortion. The mold is tapered to follow the shrinkage of the steel strand to prevent excessive gaps from forming between the mold wall and shell surface, as well as preventing bulging of the shell. Linear taper is defined by providing the percentage per meter as follows:

$$d_{taper} = \frac{(\% Taper/m)}{100} \frac{W}{2} v_c t$$
(4.38)

where W, v_c and t are the mold width, casting speed and current time below meniscus, respectively. As the modelled section of the steel strand moves down from the meniscus, the mold wall distorts away from the solidifying shell, and tapers towards it. Mold distortion arises from two main sources, thermal expansion of the mold wall due to heating during operation, and mold wear due to friction between the mold and the strand. For the billet casting simulation presented here, mold distortion is considered to be simple thermal expansion as follows, ignoring residual distortion and mold wear.

$$d_{molddist} = \alpha_{mold} \frac{W}{2} (\bar{T} - \bar{T}_0) \tag{4.39}$$

where \overline{T} is the average temperature through the mold wall thickness as a function of the distance below mold exit. \overline{T}_0 is the average mold wall temperature where the solid shell begins, α_{mold} is the thermal expansion coefficient of the copper mold tube, and W is section width.

Arbitrary complex mold shapes can be modelled by providing an external data file or function with mold wall positions at different distances below the meniscus, and even around the perimeter. For example, complex 3-D mold distortion profiles [38] are used for slab casting simulations with CON2D [19,80].

4.6.2 Contact Algorithm for Shell Surface Constraint

The mold wall provides support to the solidifying shell before it reaches the mold exit. A proper mold wall constraint is needed to prevent the solidifying shell from penetrating the mold wall, while also allowing the shell to shrink freely. Because the exact contact area between the mold wall and the solidifying shell is not known aprior, an iterative solution procedure is needed.

Some early finite element models solved contact problems by the Lagrange multiplier approach, which introduces new unknowns to the system as well as numerical difficulties [162]. This work adopts a penalty method developed by Moitra [19,80] which is tailored to this particular casting problem domain. It solves the contact problem only approximately, but is easy to implement and is more stable. Iteration within a time step proceeds as follows. At first, the shell is allowed to deform freely without mold constraint. Then, the intermediate shell surface is compared to the current mold wall position. A fraction of all penetrated nodes, identified by Equation 4.40, are restrained back to the mold wall position by a standard penalty method, and the stress simulation is repeated.

$$\{u\} \cdot \hat{n} - d_{wall} < -d_{pen} \tag{4.40}$$

where d_{pen} is the specified penetration tolerance. Iteration continues until no penetration occurs.

The nodes to be constrained are chosen by checking three scenarios shown in Figure 4.5:

- 1. In Figure 4.5a, a portion of the shell surface with length L penetrates the mold, and the maximum penetration is found at the centerline of the strand face. Those shell boundary nodes in the half of this violated length nearest to the face center, L_c , are constrained in the next iteration.
- 2. In Figure 4.5b, the center of the shell surface penetrates the mold but does not penetrate the most. Those violated nodes from the maximum penetration position to the face center are constrained in the next iteration.
- 3. In Figure 4.5c, the center of the shell surface does not penetrate the mold. That half of the violated nodes closest to the face center are constrained in the next iteration.

Commercial software, such as ABAQUS, generally constrains violated nodes one by one until convergence is reached. The present method is believed to be more computationally efficient for the particular quarter mold and behavior of interest in this work. The friction between the shell and mold surface is ignored in this model. This would need to be added to consider phenomena such as transverse cracks due to excessive taper.

4.7 Solidification Front Treatment

4.7.1 Superheat Flux

Superheat is the amount of heat stored in the liquid steel that needs to be extracted before it reaches the liquidus temperature. Superheat is treated in one of two ways:

- 1. Heat conduction method.
- 2. Superheat flux method.

The heat conduction method simply sets the initial steel temperature to the pouring temperature, and increases the conductivity of the liquid by 6.5 times to crudely approximate the effects of fluid flow [163]. This method evenly distributes the superheat over the solidification front. In reality, the superheat distribution is uneven due to the flow pattern in the liquid pool.

The second method first obtains the superheat flux distribution from a separate fluid flow computation, such as done previously for billets [164] or slabs [165]. This superheat flux at a given location on the strand perimeter is applied to appropriate nodes on the solidification front. Specifically, it is applied to the two nodes just below the liquidus in those 3-node elements with exactly one node above the liquidus. This is shown in Figure 4.6, where the isotherm is the liquidus. The initial liquid temperature is set just above the liquidus, to avoid accounting for the superheat twice.

4.7.2 Ferrostatic Pressure

Ferrostatic pressure greatly affects gap formation by encouraging contact between the shell and mold, depending on the shell strength. The ferrostatic pressure is calculated by:

$$F_p = \rho g z \tag{4.41}$$

where z is distance of the current slice from the meniscus found from the casting speed and the current time. Ferrostatic pressure is treated as an internal load that pushes the shell toward the mold wall, as shown in Figure 4.6. It is applied equally to those two nodes just below the coherency temperature that belong to those 3-node elements having exactly one of its 3 nodes above the $T_{coherency}$ isotherm. It is assembled to the global force vector through Equation B.11 in Appendix B, which gives:

$$\{F_{fp}\} = \sum_{movingboundary elements} \left\{ \begin{array}{c} \frac{F_p L_{ij}}{2} \\ \frac{F_p L_{ij}}{2} \end{array} \right\}$$
(4.42)

where L_{ij} is the boundary length between node *i* and *j* within a 3-node element.

4.8 Implementation of the Hot Tear Criterion under Complex Strain State

To predict hot tear cracks based on stress and strain histories, the model accumulates "damage strain" at every node in the grid by summing the flow strain and elastic strain components during the time steps when the nodal temperature is in the brittle temperature range, ΔT_B . This is reasonable to compare to the critical strain (Equation 2.1) from measured total strain because the flow strain and elastic strain dominate the total strain in the mushy zone. The "damage strain" provides a relative measure of crack potential.

Furthermore, comparing the appropriate damage strain component with the critical strain given in Equation 2.1 allows the model to predict crack formation and even crack orientation. Equation 2.1 provides a scalar critical strain as the crack threshold value to be compared with. However, the strain state is described by a multi-dimensional tensor. The proper component to compare to the critical strain must be chosen.

As discussed in Section 2.2, hot tear cracks initiate due to insufficient liquid feeding into the interdendritic space under thermal and mechanical deformation [3, 81–86]. For columnar dendrite structures which are always encountered in the continuous casting of steel, the direction perpendicular to the primary dendrite arms is the weakest direction of the columnar dendrite structure. Therefore, the damage strain component perpendicular to the primary dendrite arms is chosen as the state variable to compare to the critical strain in this work. For the same reason, the strain rate used in Equation 2.1 to calculate the critical strain should also be taken as the value of the strain rate component perpendicular to the primary dendrite arms.

4.8.1 Hot Tear Criterion in CON2D

In the transverse section domain modelled by CON2D, the strain and strain rate component chosen is straightforward as there is only one strain or strain rate component perpendicular to the primary dendrite arms in 2-D space. It is often reasonable to assume that dendrites grow along the temperature gradient direction along which the temperature decreases the fastest. Then, the hot tear criterion is implemented as follows:

1. Calculate the current temperature gradient ∇T based on heat transfer model results as

$$\nabla T = [B] \left\{ \begin{array}{c} T_1 \\ T_2 \\ T_3 \end{array} \right\}$$
(4.43)

where T_1 , T_2 , T_3 are the nodal temperature of the 3-node heat transfer elements and [B] is their global B matrix given in Equation A.2. The direction of decreasing temperature gradient is considered to be the growth direction of primary dendrite arms, d_1 .

$$\boldsymbol{d}_1 = -\nabla T = \{d_{1x}, d_{1y}\}^T \tag{4.44}$$

2. Find out the unit vector, d_2 , which is perpendicular to the primary dendrite arms by solving the following equations for d_2 .

$$\boldsymbol{d}_1 \cdot \boldsymbol{d}_2 = 0 \tag{4.45}$$

$$\| \boldsymbol{d}_2 \| = \left(d_{2x}^2 + d_{2y}^2 \right)^{\frac{1}{2}} = 1$$
 (4.46)

3. At the end of each time step, calculate the incremental strain and strain rate component perpendicular to the temperature gradient direction for those element Gauss points within the brittle temperature range, whose fraction of solid is between 90% and 99%.

$$\Delta \epsilon_{htc} = (\boldsymbol{d}_2)^T \cdot \Delta t \dot{\boldsymbol{\epsilon}}^{in} \cdot \boldsymbol{d}_2 \quad , 0.9 \le f_s \le 0.99 \tag{4.47}$$

$$\dot{\epsilon}_{htc} = (\boldsymbol{d}_2)^T \cdot \dot{\boldsymbol{\epsilon}}^{in} \cdot \boldsymbol{d}_2 \quad , 0.9 \le f_s \le 0.99 \tag{4.48}$$

4. Calculate hot tear damage strain $\epsilon_{hot-tear}$ by accumulating all of the incremental strain between 90% and 99% solid.

$$\epsilon_{hot-tear} = \sum_{f_s=0.9}^{f_s=0.99} \Delta \epsilon_{htc} \tag{4.49}$$

- 5. Calculate the critical strain ϵ_c by Equation 2.1. Note that the strain rate used in Equation 2.1 is the average strain rate within the brittle temperature range.
- 6. Hot tear cracks are assumed to initiate when $\epsilon_{hot-tear} \geq \epsilon_c$.

4.8.2 Hot Tear Criterion in a 3-D Model

This hot tear criterion is extended to 3-D thermal stress models. The procedure is the same as described in the last section for the 2-D model. However, there are infinite number of directions could satisfy the condition of being perpendicular to a given direction in a 3-D space. Thus, a sweeping procedure is needed to go over large enough number of directions

around the given temperature gradient direction to choose the direction which has the largest tensile strain magnitude. This direction is the most cracking suspect direction. Then, the incremental strain component to be accumulated into the damage strain and the strain rate component used in Equation 4.49 is along this direction.

The general algorithm is described as below in summary:

1. Calculate the temperature gradient as

$$\nabla T = \begin{bmatrix} \frac{\partial T}{\partial x} \\ \frac{\partial T}{\partial y} \\ \frac{\partial T}{\partial z} \end{bmatrix} = \mathbf{J}^{-1} \mathbf{B} \mathbf{T} = \begin{bmatrix} \frac{\partial x}{\partial g} & \frac{\partial y}{\partial g} & \frac{\partial z}{\partial g} \\ \frac{\partial x}{\partial h} & \frac{\partial y}{\partial h} & \frac{\partial z}{\partial h} \\ \frac{\partial x}{\partial r} & \frac{\partial y}{\partial r} & \frac{\partial z}{\partial r} \end{bmatrix}^{-1} \begin{bmatrix} \frac{\partial N_1}{\partial g} & \frac{\partial N_2}{\partial g} & \cdots & \frac{\partial N_{\#node}}{\partial g} \\ \frac{\partial N_1}{\partial h} & \frac{\partial N_2}{\partial h} & \cdots & \frac{\partial N_{\#node}}{\partial h} \\ \frac{\partial N_1}{\partial r} & \frac{\partial N_2}{\partial r} & \cdots & \frac{\partial N_{\#node}}{\partial r} \end{bmatrix} \begin{bmatrix} T_1 \\ \vdots \\ T_{\#node} \end{bmatrix}$$
(4.50)

where $\sharp node = 8$ for a 3-D linear brick element. The direction of decreasing temperature gradient is considered to be the growth direction of primary dendrite arms, d_3 .

$$\boldsymbol{d}_3 = -\nabla T = \{d_{3x}, d_{3y}, d_{3z}\}^T \tag{4.51}$$

- 2. Chose the directions perpendicular to the temperature gradient direction. The normalized sampling directions, d_{si} , are chosen to equally distribute around the temperature gradient direction with 5° interval. Only half of directions in the circle around the temperature gradient direction (180°) are considered due to the equal strain magnitude between the two opposite directions. The detail of the sweeping algorithm is in Appendix C.
- 3. Project the incremental inelastic strain and strain rate to each sweeping direction d_{si} within the brittle temperature range, whose fraction of solid is between 90% and 99%.

$$\epsilon_{htci} = (\boldsymbol{d}_{si})^T \cdot \Delta \boldsymbol{\epsilon}^{in} \cdot \boldsymbol{d}_{si} \quad , 0.9 \le f_s \le 0.99 \tag{4.52}$$

$$\dot{\epsilon}_{htci} = (\boldsymbol{d}_{si})^T \cdot \dot{\boldsymbol{\epsilon}} \cdot \boldsymbol{d}_{si} \quad , 0.9 \le f_s \le 0.99 \tag{4.53}$$

4. Choose hot tear damage strain to be the largest tensile strain magnitude from all sample directions.

$$\epsilon_{hot-tear} = max(\epsilon_{htc1}, \dots, \epsilon_{htcn}) \tag{4.54}$$

where n(=36) is the total number of the sweeping directions.

5. Hot tear crack initiate when $\epsilon_{hot-tear} \geq \epsilon_c$, where the critical strain ϵ_c is calculated by Equation 2.1.

A joint activity was initiated between the Metal Processing Lab at the University of Illinois and Champaign Simulation Center of Caterpillar (CSC) Corporation. A couple of commercial packages are involved during the simulation of casting process at CSC. Temperature field is calculated by heat transfer and solidification packages such as MAGMA. Then, the temperature distribution is imported into ABAQUS to perform thermal-stress analysis to obtain residue stresses and strains. The 3-D version of the hot tear criterion is implemented as an add-on program under ABAQUS frame to further post-process ABAQUS result file (odb file) in order to predict hot tear cracks.

4.9 Mechanical Properties

This work adopts temperature-dependent steel properties chosen to be as realistic as possible.

4.9.1 Phase Fraction Model

A non-equilibrium pseudo-binary Fe-C phase diagram abstracted from a micro-segregation model for plain carbon steels [166] is incorporated in CON2D to approximate the realistic phase fraction evolution between the solidus and liquidus temperatures. Figure 4.7 shows the non-equilibrium pseudo-binary Fe-C phase diagram in which points A through H are taken from the simple micro-segregation model [166]. This phase diagram is constructed for the carbon steel with 1.52%Mn, 0.34%Si, 0.012%P , and 0.02%S at the cooling rate of 10 $K \cdot sec.^{-1}$ and the arm spacings given in [167].

The extra chemical components and the fast cooling rate make the peritectic reaction conduct over a temperature range rather than a single temperature. Thus, point F is located below the peritectic temperature indicated by points D and E. This phase diagram is an isopleth [168] of a more complex multi-component phase diagram which typically has up to 14 dimensions representing the 13 chemical elements and temperature along each dimension. For example if only one extra chemical element, Si, was added into the Fe-C system, a ternary phase diagram with Fe, C, and Si at its three vertices would be needed to determine the phase fractions at any given temperature in the triangle DEF. To do this properly requires consideration of the point, P, within the Fe-C-Si triangle that represents an alloy with specific Fe, C, and Si content. The amount of each component is determined by the distance between P and vertices corresponding to that component. When the point P lies within a two phase or a three phase region, the phase fractions can be determined by the lever rule across the multi-dimensional tie line between the internal boundaries of the multi-phase region. Unfortunately, the already complex ternary phase diagram is still much too simple to evaluate the real alloys. Even advanced numerical models, such as ThermoCalc [169], have difficulty to accurately calculate the phase fractions from a multi-dimensional phase diagram.

To simplify the issue, it is assumed in this work that the peritectic austenite(γ) phase evolutes linearly from the starting temperature of the peritectic reaction (determined by the line between points D and E) to the ending temperature of the pertectic reaction (determined by the lines DF and FE). On the lines DF and FE, there are the mixture phases of $\delta + \gamma$ and liquid+ γ , respectively. Their fractions can be determined by the lever rule within the three phase triangle, DFE. In addition to the assumption of linear evolution of γ from the beginning to the end of the peritectic reaction, All the fractions of δ , γ , and liquid can be determined. Figure 4.7 also compares the 100% and 75% solid lines produced by this pseudo-binary phase diagram with the ZST and ZDT measurements by Schmidtmann *et. al.* [167]. Figure 4.8 shows the evolution of the fractions of solid, δ -ferrite, and austenite for the four carbon steels (0.003%C, 0.044%C, 0.1%C, 0.27%C, and 0.44%C) from their liquidus to their solidus. It can be seen that the phase fractions during solidification produced by the pseudo-binary phase diagram are fairly close to those produced by the more comprehensive micro-segregation model [166], especially for the liquid fraction which is of most important to this work.

4.9.2 Thermal Properties

The temperature dependent conductivity function for plain carbon steel is fitted from measured data compiled by K. Harste [170] and is given in Equation 4.55. Figure 4.9 shows the conductivity for several typical plain carbon steels. The conductivity increases linearly through the mushy zone to the liquid by a factor of 6.5 to partly account for the effect of convection due to flow in the liquid steel pool [163] if the heat conduction method is chosen. If the superheat flux method as described in Section 4.7.1 is chosen, the conductivity in the liquid and mushy zone will not be increased.

$$K(W/mK) = K_{\alpha}f_{\alpha} + K_{\delta}f_{\delta} + K_{\gamma}f_{\gamma} + K_{l}f_{l}$$
where
$$K_{\alpha} = [80.91 - 9.9269 \times 10^{-2}T(^{o}C) + 4.613 \times 10^{-5}T(^{o}C)^{2}][1 - a_{1}(\%C)^{a_{2}}]$$

$$K_{\delta} = [20.14 - 9.313 \times 10^{-3}T(^{o}C)][1 - a_{1}(\%C)^{a_{2}}]$$

$$K_{\gamma} = 21.6 - 8.35 \times 10^{-3}T(^{o}C)$$

$$K_{l} = 39.0$$

$$a_{1} = 0.425 - 4.385 \times 10^{-4}T(^{o}C)$$

$$a_{2} = 0.209 + 1.09 \times 10^{-3}T(^{o}C)$$
(4.55)

The enthalpy curve used to relate heat content and temperature in this work, H(T), is obtained by integrating the specific heat curve $c_p(T)$ fitted from measured data compiled by K. Harste [170] as given in Equation 4.55. Figure 4.10, shows the enthalpy for the typical plain carbon steels.

$$H(KJ/Kg) = H_{\alpha}f_{\alpha} + H_{\delta}f_{\delta} + H_{\gamma}f_{\gamma} + H_{l}f_{l}$$
where
$$H_{phase} = [b_{-1}T(K)^{-1} + b_{0} + b_{1}T(K)^{1} + b_{2}T(K)^{2} + b_{3}T(K)^{3}]a_{phase}(\%C)$$
(4.56)

The parameter values and the carbon content dependent functions, a, for all phases are listed in Tables 4.2 and 4.3.

For the multi-phase region, both conductivity and enthalpy are calculated by weighted averaging of their different phase values using their volume fraction, f. The subscripts (α , δ , γ , and l) in Equations 4.55 and 4.56 are represent for δ -ferrite, α -ferrite, austenite and liquid, respectively. The subscript, *phase*, in Equation 4.56 represents one of the four phase, α , δ , γ , or l.

4.9.3 Thermal Linear Expansion

The thermal linear expansion function is obtained from solid phase density measurements compiled by K. Harste [170] and Jablonka [171] and liquid density measurements by Jimbo and Cramb [172].

$$TLE = \sqrt[3]{\frac{\rho(T_0)}{\rho(T)}} - 1$$
where
$$\rho(Kg/m^3) = \rho_{\alpha}f_{\alpha} + \rho_{\delta}f_{\delta} + \rho_{\gamma}f_{\gamma} + \rho_lf_l$$

$$\rho_{\alpha} = 7881 - 0.324T(^{o}C) - 3 \times 10^{-5}T(^{o}C)^2 \qquad (4.57)$$

$$\rho_{\delta} = \frac{100[8011 - 0.47T(^{o}C)]}{[100 - (\%C)][1 + 0.013(\%C)]^3}$$

$$\rho_{\gamma} = \frac{100[8106 - 0.51T(^{o}C)]}{[100 - (\%C)][1 + 0.008(\%C)]^3}$$

$$\rho_l = 7100 - 73(\%C) - [0.8 - 0.09(\%C)][T(\%C) - 1550]$$

A simple mixture rule is applied to obtain the density value from the values of different phases. The subscripts in Equation 4.57 have the same meaning as in Equations 4.55 and 4.56. Figure 4.11 shows the thermal linear expansion curves for the typical plain carbon steels.

4.9.4 Inelastic Constitutive Properties

The unified constitutive model developed here uses the instantaneous equivalent inelastic strain rate, $\dot{\epsilon}_{in}$, as the scalar state function, which depends on the current equivalent stress, $\bar{\sigma}$, temperature, T, the current equivalent inelastic strain, $\bar{\epsilon}_{in}$, which accumulates below the coherent temperature, and the carbon content of the steel [58,59,66]. The model is developed to match tensile test measurements of Wray [58] and creep test data of Suzuki [62]. Model III by Kozlowski given in Equation 4.58 is adopted to simulate the mechanical behavior of austenite.

$$\begin{split} \dot{\epsilon}_{pl-\gamma}(sec^{-1}) &= Cexp\left(\frac{-Q}{T}\right)|F|^{n-1}F\\ where\\ F &= \bar{\sigma} - a_{\epsilon}|\bar{\epsilon}_{in}|^{n_{\epsilon}-1}\bar{\epsilon}_{in}\\ Q &= 4.465 \times 10^{4}\\ C &= 4.655 \times 10^{4} + 7.14 \times 10^{4}(\% C) + 1.2 \times 10^{5}(\% C)^{2}\\ a_{\epsilon} &= 130.5 - 5.128 \times 10^{-3}T\\ n_{\epsilon} &= -0.6289 - 1.114 \times 10^{-3}T\\ n &= 8.132 - 1.54 \times 10^{-3}T \end{split}$$
(4.58)

The equivalent stress $\bar{\sigma}$ is calculated as

$$\bar{\sigma} = c \left(\frac{3}{2} \boldsymbol{\sigma}' : \boldsymbol{\sigma}'\right)^{\frac{1}{2}}$$
where
$$c = \begin{cases} \frac{\sigma_{max}}{|\sigma_{max}|} & |\sigma_{max}| \ge |\sigma_{min}| \\ \frac{\sigma_{min}}{|\sigma_{min}|} & |\sigma_{max}| < |\sigma_{min}| \end{cases}$$

$$\sigma_{max} = max(\sigma_{11}, \sigma_{22}, \sigma_{33})$$

$$\sigma_{min} = min(\sigma_{11}, \sigma_{22}, \sigma_{33})$$
(4.59)

where σ_{11} , σ_{22} , and σ_{33} are the principal stresses.

A power law model is developed to model the behavior of δ -ferrite [20], given as follows:

$$\dot{\bar{\epsilon}}_{pl-\delta}(sec^{-1}) = C |\bar{\sigma}|^{n-1} \bar{\sigma}(1+1000 |\bar{\epsilon}_{in}|)^{mn}$$
where
$$C = 0.1 \left(\frac{(T/300)^{5.52}}{1.3678 \times 10^4 (\%C)^{-5.56 \times 10^{-2}}} \right)^n$$

$$m = 9.4156 \times 10^{-5}T - 0.349501$$

$$n = (1.617 \times 10^{-4}T - 0.06166)^{-1}$$
(4.60)

Figure 4.12 compares the stresses measured by Wray [58] to those predicted by the constitutive models at 5% strain under different strain rates. The constitutive models give

acceptable performance. This figure also shows that δ -ferrite, which forms at higher temperatures found near the solidification front, is much weaker than austenite. This greatly affects the mechanical behavior of the solidifying steel shell.

A simple mixture rule is not appropriate in two-phase regions that contain interconnecting regions of a much weaker phase. Thus, the constitutive model given in Equation 4.60 is applied in the solid whenever the volume fraction of ferrite (δ -ferrite above 1400°C, δ -ferrite below 900°C) is more than 10%. Otherwise, Equation 4.58 is adopted.

To make the constitutive model properly handle kinematic hardening during reverse loading, the equivalent stress/strain used in Equations 4.58 and 4.60 are given the same sign as the principal stress/strain having the maximum magnitude. The inelastic strain rate, as a consequence, also bears a sign.

Two uniaxial tensile experiments [21,59] and a creep experiment [62] on plain carbon steel at elevated temperatures are simulated by CON2D to test the performance of its constitutive models. Figures 4.13 and 4.14 show CON2D predictions of tensile test behavior of austenite and δ -ferrite at constant strain rate around $10^{-4}s^{-1}$ which is typically encountered in the shell during continuous casting [59]. The results also compare reasonably with experiments at small strain (< 5%), although they over-predict the stress when the strain exceeds 5%. Because the strain generally stays within 5% for the entire continuous casting process, the constitutive models are quite reasonable for this purpose. Figure 4.15 shows the CON2D predictions of creep test behavior at constant load. The inelastic strain predictions match the measurements reasonably well, especially at times shorter than 50 seconds, of most concern to continuous casting in the mold region. Beyond this time, CON2D under-predicts creep, which is consistent with the over-prediction of stress, observed in the tensile test cases. Monotonic loading is unlikely beyond this length of time, anyway. Figure 4.16 compares CON2D predictions and creep test measurements [62] under a sinusoidal alternating load with full reversal (R-ratio = 1.167). Although more measurements and computations of complex loading conditions would be helpful, these comparisons show that the constitutive models in CON2D are reasonable, even for conditions that include reverse loading.

4.9.5 Elastic Properties

The temperature-dependent elastic modulus curve used in this model is a stepwise linear fit of measurements by Mizukami *et. al.* [173] given in Figure 4.17. Unlike in some other models, the elastic modulus of the liquid here is given the physically realistic value of 10GPa. Poisson ratio is 0.3 constant. Measurements of higher Poisson ratios at high temperature are attributed to creep occurring during the experiment. Incorrectly incorporating part of the volume conserved plastic behavior, where $\nu = 0.5$, into the elastic ν will cause numerical difficulty for the solver.

4.10 Model Validation

An analytical solution of thermal stress model in an unconstrained solidifying plate, derived by Weiner and Boley [4] is used here as an ideal validation problem for solidification stress models. Constants for this validation problem chosen here to approximate the conditions of interest in this work are listed in Table 4.4.

The material in this problem has elastic-perfect plastic behavior. The yield stress drops linearly with temperature from 20MPa at $1000^{\circ}C$ to 0MPa at the solidus temperature $1494.35^{\circ}C$. For the current elastic-viscoplastic model, this constitutive relation is transformed into a computationally more challenging form, the highly nonlinear creep function of Equation 4.14 with $A = 1.5 \times 10^8$ and $\sigma_{yield} = 0.01MPa$ in the liquid. A very narrow mushy region, $0.1^{\circ}C$, is used to approximate the single melting temperature assumed by Boley and Weiner. In addition to the generalized plane strain condition in the axial z-direction, a similar condition is imposed in the y-direction (parallel to the surface) by coupling the displacements of all nodes along the top surface of the slice domain as shown in Figure 4.24. The analytical solutions are computed with MATLAB [174]. Figures 4.18 and 4.19 show the temperature and the stress distributions across the solidifying shell at different solidification times using an optimized mesh and time step, similar to that adopted for the 2-D billet casting simulation. The mesh is gradually increased in size from 0.3mm at the left end to 2.0mm at right end, and time step size is increased from 0.001sec. at the beginning to 0.1sec. at the end.

Figures 4.20 \sim 4.23 show the relative average errors, given in Equation 4.61 for the temperature and stress predictions, respectively.

$$Error_{T}(\%) = \frac{\sum_{1}^{N} \sqrt{\left(T_{i}^{CON2D} - T_{i}^{Analytical}\right)^{2}}}{\frac{N|T_{melt} - T_{cold}|}{\sigma_{i}^{CON2D} - \sigma_{i}^{Analytical}}} \times 100$$

$$Error_{\sigma}(\%) = \frac{\sum_{1}^{N} \sqrt{\left(\sigma_{i}^{CON2D} - \sigma_{i}^{Analytical}\right)^{2}}}{\frac{N|\sigma(T_{melt}) - \sigma(T_{cold})|}{\gamma(\sigma_{i}^{CON2D})}} \times 100$$
(4.61)

Accuracy of the CON2D predictions increases if the mesh and time step are refined together. A fine uniform mesh of 0.1mm, with small uniform time step of 0.001sec., produces relative average errors within 1% for temperature and within 2% for stress. However, the computational cost is also high. Note that the inaccuracy is severe at early times of the simulation, especially for the stress predictions. This is because the solidified layer initially spans only a few elements. As the solid portion of the plate grows thicker, the mesh size and time step requirements become less critical. Thus, a non-uniform mesh with increasing time step size is better to satisfy both accuracy and efficiency. The optimal choice, used in Figures 4.18 and 4.19, gives a decent prediction with the relative average errors within 2% for temperature and 3% for stress. A similar mesh is adopted for the actual billet casting simulation. This demonstrates that the model is numerically consistent and has an acceptable mesh.

4.11 Simulation of Billet Casting

To further validate the feature of fully coupled heat transfer and stress analysis and the contact algorithm, CON2D is next applied to simulate a plant trial conducted at POSCO,

Pohang works, South Korea [41], for a 120mm square section billet of 0.04%C steel cast at 2.2m/min, where measurements are available. The mold had a single linear taper of 0.785%/m. Details of the material and operation conditions are given in Tables 4.5 and 4.6, respectively. Two simulations are performed to predict the temperature, stress and deformation evolutions of the billet shell using the 2-D L-shaped domain (Figure 4.2) and a slice domain through the centerline of the billet face (Figure 4.24) similar to the Boley and Weiner analytical problem. The interfacial heat transfer constants for both simulations are given in Table 4.1 and are found with the help of a dedicated heat transfer code, CON1D [2].

The superheat flux profile is obtained from coupled computations of turbulent flow and heat transfer in a round billet caster by Khodadadi *et. al.* [164] for the case of Grashof number $(Gr = gW^3 (TLE(T_{pour}) - TLE(T_m))/\nu^2)$ is 1×10^8 . This value is the closest case to the current problem conditions where the Grashof number is 2×10^7 and confirms that natural convection is unimportant in this process. The heat flux is calculated from the Nusselt number, Nu, and mean liquid temperature, T_m , results given as a function of distance below meniscus [164], using their values of liquid steel conductivity, k = 29.8W/mK, mold section size, W = 200mm and $33^{\circ}C$ superheat, except for re-adjusting the superheat temperature difference as follows:

$$q_{\rm sup} = \frac{Nu \, k (T_m - T_{liq})}{W} \frac{(T_{pour} - T_{liq})_{posco}}{(T_{pour} - T_{liq})_{khod}}$$
(4.62)

where T_{pour} and T_{liq} are the pouring and liquidus temperatures, respectively. The resulting superheat flux profile is shown in Figure 4.25. Note that the total heat integrated from Figure 4.25 over the mold surface, 48.6kW, matches the superheat for the current problem, $(T_{pour} - T_{liq}) \rho c_p v_c = 46kW.$

The heat flux and mold wall temperatures predicted by CON2D along the billet face center are shown in Figures 4.26 and 4.27 respectively. These results slightly under-predict the measurements of thermo-couples embedded in the mold wall, which should lie almost exactly between the hot and cold face temperatures [40]. The total heat extracted by the mold, 128.5kW, is 17% lower than the plant measurements based on a heat balance of the mold cooling water (8K temperature rise at $9.2msec^{-1}$ slot velocity) of 154kW [41]. This is consistent with under-prediction of the mold temperatures.

The predicted shell growth for this CON2D simulation is given in Figure 4.28, as indicated by the evolution of the solidus and liquidus isotherms. This is compared with measurements of the solid-liquid interface location, obtained by suddenly adding FeS tracer into the liquid pool during steady-state casting [41]. Longitudinal and transverse sections through the billet are cut from the final product. The transverse section is 285mm from the meniscus when the FeS tracer is added. Because FeS tracer cannot penetrate the solid steel shell, sulfur prints of sections cut through the fully-solidified billet reveal the location of the solidification front and shell thickness profile at a typical instant during the process [41]. The CON2D predictions match along the centerline beyond the first 80mm below the meniscus, where the shell remains in contact the mold, suggesting that the heat transfer parameters are reasonably accurate.

The shell surface position profile down the centerline is shown in Figure 4.29, together with the mold wall position, which includes both the taper, and the mold distortion profile calculated from the CON1D temperature results using Equation 4.39 [2]. The shell surface generally follows the mold wall with no obvious penetration, validating the contact algorithm. Note, however, that a slight gap opens up within the first 25mm. Although this effect is believed to be physically reasonable owing to rapid initial shrinkage of the steel, it is exaggerated here, owing to numerical difficulties during the initial stages of solidification. This causes an over-prediction of the drop in initial heat flux and temperature observed in Figure 4.26. This drop is followed by increased heat flux (and corresponding mold wall temperature) after full contact is re-established, which has also been observed in other measurements [175].

The simulation features a detailed prediction of temperature, shrinkage, and stress in the region of the rounded billet corner. The evolution of the increases in gap size and surface temperature are given in Figures 4.30 and 4.31 near (20mm) to the centerline of the billet face and at various locations, 0, 5, 10, and 15mm, from the billet corner. The corresponding

large drops in heat flux are included in Figure 4.26. The solidifying shell quickly becomes strong enough to pull the billet corner away from the mold wall and form a gap around the corner region. The gap greatly decreases local heat flow in the corner, causing the mold wall temperature to drop.

The drop in mold temperature near the corner over the initial 80mm is more than expected in reality, because the simple mold model of CON2D in Equation 4.33 neglects heat conduction around the corner and along the casting direction. Thus, these predictions are not presented. This latter effect, which is included in CON1D [2], also contributed to the convergence difficulties along the centerline discussed in Figure 4.29. Fortunately, it has little other effect on heat flux or shell behavior.

Figure 4.30 shows how a permanent gap forms after 40mm below the meniscus, which grows to over 0.3mm thick by half-way down the mold, growing little after that. Corresponding gaps form adjacent to the corner at later times, reaching smaller maxima part-way down the mold. These gaps form because the simple linear taper of the mold walls is insufficient to match shrinkage of the shell. The corner effect decreases with distance from the corner and disappears beyond 15mm from the corner.

The corner gap and drop in heat flux causes a hot spot at the corner region, as shown in the surface temperature profiles of Figure 4.31. CON2D predicts that the shell corner reheats slightly and reaches $150^{\circ}C$ hotter than the billet face center, for the conditions of this trial. The decreased heat flux also produces less solidification in the corner, as illustrated in Figure 4.32 at 285mm below the meniscus. The predicted shell thinning around the corner is consistent with the plant measurements from the sulfur print, as quantified in Figures 4.28 and 4.32. The predictions here are also consistent with those of Park *et. al.*, who modelled how increasing billet mold corner radius leads to more severe hot and thin spots near the corner [2]. This tends to validate the CON2D model and the simple constant interfacial heat transfer parameters used to produce these results. Improving the accuracy would likely require a more complex model of gap heat transfer that considered details of surface roughness, including differences between center and corner.

Figure 4.33 shows the evolution of surface stress components near the centerline of the billet face. Stress normal to the surface (x-direction) is effectively equal to zero, which indicates that the 0.785%/m mold taper never squeezes the billet. The stress components perpendicular to the solidification direction (y-direction tangential to surface and z-casting direction) are generally very similar, which matches the behavior expected from the analytical test solution [4]. These stresses grow slowly in tension during the period of increasing heat extraction rate from 20 to 100mm below the meniscus. They reach a maximum of almost 3MPa due to the increase in shell strength at lower temperature that accompanies the transformation from δ -ferrite to austenite. This is shown in the through-thickness profile of these same stress components in Figure 4.34a, but calculated with the 1-D slice domain. The surface tensile stress peak does not penetrate very deep, owing to the very thin layer of material colder than 10% delta-ferrite. Thus, this peak might cause very shallow fine surface cracks, but nothing deeper.

The surface stresses in Figure 4.33 suddenly turn compressive beyond 100mm due to the sudden change in heat extraction rate at this distance (see Figure 4.26). Surface compression arises because the subsurface begins to cool and shrink faster than the surface. This causes a corresponding increase in subsurface tension near the solidification front that might lead to subsurface cracks. The surface stays in compression from -4 to -6MPa for the remaining time in the mold.

During the time beyond 100mm, the stress profile, Figure 4.34a, is qualitatively similar to that of the analytical test problem, as expected. Differences arise from the variation in steel strength between the δ -ferrite and austenite. Stresses in the liquid, mushy zone and δ -ferrite are always very small. Tensile stress increases rapidly during the phase transformation, which takes place at the low end of the $\delta + \gamma$ region of Figures 4.34a and 4.34c. When the δ -ferrite region is thin, this tensile stress is more likely to create strains significant to
generate cracks. These results illustrate the widely accepted knowledge that surface cracks initiate near the meniscus, while subsurface cracks form lower down.

Figures 4.34b and 4.34d show the different components of strain (y-direction) through the shell thickness near the billet face center corresponding to the stresses in Figures 4.34a and 4.34c. Thermal strains dominate in the solid and generate the other strains due to the constraint of adjacent layers of steel. Small elastic strains are generated by the mismatch of thermal strain, although the stresses they generate may still be significant. Inelastic strain is generated in regions of high-stress, starting in the $\delta + \gamma$ region. It is high at the surface at the top of the mold and later grows in the austenite. Note that inelastic strains are all tensile throughout the shell. The δ and mushy zones behave elastically with very low stresses. This is fortunate as these phases are very weak and cannot accommodate much inelastic strain before cracking. Flow strain in the liquid occurs to accommodate the total strain, which is naturally flat, owing to the constraint by the solid.

Figure 4.35 shows the "hoop" stress component (y direction parallel to billet surface and perpendicular to casting direction) at an off-corner location (10mm above the billet corner) through the shell thickness at 100mm, 500mm, and 700mm (mold exit) below meniscus. Stresses all behave similarly to the corresponding locations along the billet centerline, except that the tension and compression are lower. This is expected due to the slower cooling rates, shallower temperature gradients, and higher temperatures near the corner.

Figures 4.36 and 4.37 show contours of the stress and inelastic strain components perpendicular to the solidification direction superimposed on the distorted billet at mold exit with isotherms. The insufficient 0.785%/m taper of this mold is unable to support the billet which allows a slight bulge (0.25mm at mold exit). Regions of high tensile stress and inelastic strain are indicated at the off-corner subsurface ($10 \sim 20mm$ from the corner and $2 \sim 6mm$ beneath the surface).

4.12 Figures and Tables



Fig. 4.1: Schematic of the modeling domain of casting billet



Fig. 4.2: L-shape mesh with 3-node heat transfer and 6-node stress elements



Fig. 4.3: Schematic of thermal resistor model of the interfacial layer between mold and shell surface



Fig. 4.4: CON2D flow chart



Fig. 4.5: Three types of penetration modes in contact algorithm



Fig. 4.6: Schematic of the moving front tracking method



Fig. 4.7: Non-equilibrium Fe-C phase diagram predicted by the microsegregation model used in CON2D (other components: 1.52%Mn, 0.34%S, 0.02%S, 0.012%P)



Fig. 4.8: Evolution of the fractions of solid, δ -ferrite, and austenite from liquidus to solidus for the six carbon steels investigated in this work (other components: 1.52%Mn, 0.34%S, $0.02\%S, 0.012\%P)_{98}$



Fig. 4.9: Conductivity of plain carbon steels



Fig. 4.10: Enthalpy of plain carbon steels



Fig. 4.11: Thermal linear expansion (TLE) of plain carbon steels



Fig. 4.12: Comparison of CON2D predicted and measured stress (Wray) at 5% plastic strain



Fig. 4.13: CON2D prediction of the stress-strain relation of steel compared with measurements for uniaxial tensile test up to 1400 oC



Fig. 4.14: CON2D prediction of the stress-strain relation of steel compared with measurements for uniaxial tensile test above 1400 oC



Fig. 4.15: CON2D prediction of the stress-strain relation of steel compared with measurements for creep test at elevated temperature



Fig. 4.16: CON2D prediction of the stress-strain relation of steel compared with cyclic loading condition at elevated temperature



Fig. 4.17: Elastic modulus for plain carbon steels used in CON2D



Fig. 4.18: Temperature profiles through an infinite solidifying plate at different solidification times comparing with Boley and Weiner analytical solution [4]



Fig. 4.19: Stress profiles through an infinite solidifying plate at different solidification times comparing with Boley and Weiner analytical solution [4]



Fig. 4.20: Time step size effect to CON2D temperature prediction



Fig. 4.21: Time step size effect to CON2D stress prediction



Fig. 4.22: Mesh refinement effect to CON2D temperature prediction



Fig. 4.23: Mesh refinement effect to CON2D stress prediction



Fig. 4.24: Schematic of slice domain at the billet centerline



Fig. 4.25: Superheat flux used in CON2D for billet casting simulation



Fig. 4.26: Predicted instantaneous heat flux profiles in billet casting mold



Fig. 4.27: Predicted mold wall temperature profiles compared with plant measurements



Fig. 4.28: Predicted shell thickness profiles for billet casting compared with plant measurements



Fig. 4.29: Mold distortion, mold wall position and shell surface profiles for the billet casting simulation



Fig. 4.30: Gap evolution predicted by CON2D for the billet casting simulation



Fig. 4.31: Shell surface temperatures predicted for billet casting simulation



Fig. 4.32: Temperature contours at 285mm below meniscus compared with corresponding sulfur print from plant trial



Fig. 4.33: Surface stress histories predicted near the billet face center (2-D L-mesh domain)



Fig. 4.34: Stress, temperature and strains predicted through the shell thickness far from billet corner (slice domain)



Fig. 4.35: Stress predicted through the shell thickness near billet corner (2-D L-mesh domain)



Fig. 4.36: Stress contours predicted at mold exit



Fig. 4.37: Inelastic strain contours predicted at mold exit

Table 4.1: Parameters in the heat resistor model

| Cooling water heat transfer coefficient, $h_{water}(W/m^2K)$ | 22000 25000 |
|--|----------------------|
| Cooling water temperature, $T_{water}(^{o}C)$ | 30 42 |
| Mold wall thickness, $t_{mold}(mm)$ | 6 |
| Mold wall conductivity, $k_{mold}(W/mK)$ | 360 |
| Gap conductivity, $k_{gap}(W/mK)$ | 0.015 |
| Contact resistance, $r_{contact}(m^2 K/W)$ | 7.5×10^{-4} |
| Mold wall emissitivity, ε_m | 0.5 |
| Steel emissitivity, ε_s | 0.8 |

Table 4.2: Value of the parameters in enthalpy equation 4.56

| | Phase | b_{-1} | b_0 | b_1 | b_2 | b_3 |
|----------|---------------------|-------------------------|-----------------------|----------------------|-------------------------|----------------------|
| α | $T \le 800$ | 5188 | -86 | 0.505 | -6.55×10^{-5} | 1.5×10^{-7} |
| | $800 < T \le 1000$ | -1.11×10^{6} | 4056 | -4.72 | 2.29×10^{-3} | 0 |
| | $1000 < T \le 1042$ | 0 | 5780 | -11.5 | 6.238×10^{-3} | 0 |
| | $1042 < T \le 1060$ | 0 | -18379 | 34.87 | -0.016013 | 0 |
| | $1060 < T \le 1184$ | -5.1766×10^{6} | 12822 | -10.068 | 2.9934×10^{-3} | 0 |
| | δ | 0 | 5.09×10^{4} | 4.41×10^{2} | 8.87×10^{-2} | 0 |
| | γ | 0 | 9.35×10^4 | 4.30×10^2 | 7.49×10^{-2} | 0 |
| | l | 0 | -1.05×10^{5} | 8.25×10^2 | 0 | 0 |

Table 4.3: Carbon content function in the enthalpy equation 4.56

| α | 1 |
|----------|---|
| δ | $[18(\%C) + 2.0 \times 10^{3}(\%C)^{2}][44(\%C) + 1200]^{-1}$ |
| γ | $[37(\%C) + 1.9 \times 10^{3}(\%C)^{2}][44(\%C) + 1200]^{-1}$ |
| l | 1 |

Table 4.4: Constants used in Boley and Weiner analytical solution

| Conductivity (W/mK) | 33.0 |
|--|---------|
| Specific heat (kJ/kgK) | 0.661 |
| Latent heat (kJ/kg) | 272.0 |
| Elastic modulus in Solid (GPa) | 40.0 |
| Elastic modulus in Liquid (GPa) | 14.0 |
| Thermal linear expansion coefficient $(1/K)$ | 0.00002 |
| Density (kg/m^3) | 7500.0 |
| Poisson's ratio | 0.3 |
| Melting temperature (^{o}C) 1494.4 | |
| Liquidus temperature (^{o}C) | 1494.45 |
| Solidus temperature (^{o}C) | 1494.35 |
| Cold surface temperature (^{o}C) | 1000.0 |

Table 4.5: Material details in billet plant trial at POSCO

| Steel composition $(wt\%)$ | 0.04C |
|--|--------|
| Liquidus temperature (^{o}C) | 1532.1 |
| 70% Solid temperature (°C) | 1525.2 |
| 90% Solid temperature (°C) | 1518.9 |
| Solidus temperature (^{o}C) | 1510.9 |
| Austenite rightarrow α -ferrite starting temperature (°C) | 781.36 |
| Eutectoid temperature (^{o}C) | 711.22 |

Table 4.6: Simulation conditions in billet plant trial at POSCO

| Billet section size $mm \times mm$ | 120×120 |
|--|--------------------------------------|
| Working mold length mm | 700 |
| Total mold length mm | 800 |
| Casting speed (m/min) | 2.2 |
| Mold corner radius (mm) | 4 |
| Taper $\%/m$ | 0.785 (on both faces) |
| Time to apply ferrostatic pressure $(sec.)$ | 2.5 |
| Mesh size $(mm \times mm)$ | $0.1 \times 0.1 \sim 1.4 \times 1.0$ |
| Number of nodes (varies with section size) | 7381 |
| Number of element (varies with section size) | 7200 |
| Time step size $(sec.)$ | $0.0001 \sim 0.005$ |
| Pouring temperature (^{o}C) | 1555.0 |
| Coherency temperature (^{o}C) | 1510.9 |
| Gap tolerance, d_{min} | $0.001 \ (0.1\%)$ |
| Minimum gap, d_{gapmin} (mm) | 0.012 |
| Penetration tolerance, d_{pen} (mm) | 0.001 |

Chapter 5. Critical Shell Thickness Due to Tensile Rupture

As indicated in Chapter 1, one of the phenomena limiting the casting speed of a caster is the excessive transverse strain due to ferrostatic pressure from the liquid steel to the thin shell. This excessive tensile strain can lead to longitudinal cracks, or "breakouts" at extreme conditions when the solidifying shell is not thick enough to withstand the ferrostatic pressure when the shell is below the mold exit.

The shell thickness at the mold exit directly depends on the amount of heat extracted by the mold. Increasing casting speed reduces the dwell time which the shell stays in the mold and total heat extracted by the mold. Thus, higher casting speed leads to thinner shell at the mold exit. Note that increasing casting speed reduces the shell thickness all over the section perimeter. In addition, there are other phenomena, such as oscillation marks, inadequate mold taper, and so on, influencing the local shell thickness. To explore the critical shell thickness, CON2D is applied to a thin section through the solidifying shell. The shell thickness at the mold exit is obtained as a function of total heat extracted by the mold regardless the cause of the heat extraction. The model tracks the evolution of temperature, solidification, stress, and strain in a slice through the solidifying shell as it moves down through the caster [59]. The model domain, illustrated in Figure 5.1, is a slice through the solidifying shell at the center of one side of the continuous cast strand. This slice domain is 0.2mm thick and has a maximum length of half of the strand section size. A fine mesh of 10 nodes per mm is used to achieve acceptable accuracy. This mesh is connected into 3-node and 6-node triangle elements for heat transfer and stress analysis, respectively.

The effects of ferrostatic pressure are modelled by applying a force onto the edges of the solidifying shell domain. This force, F, is evaluated with Equation 5.1, which balances the stress across the shell at every distance, z(m), below the mold exit with the local ferrostatic

pressure, $\rho(Kgm^{-3})g(ms^{-2})z(m)$.

$$F(Nm^{-1}) = \rho g z (W - 2b)/2 \tag{5.1}$$

where W(m) is the slab thickness for slab casting or the section size for billet casting, and b(m) is the shell thickness as shown in Figure 5.1.

5.1 Heat Flux Profile

The average heat transfer rate over the continuous casting mold has been measured to drop with time, as illustrated in Figure 5.2 [5–8]. These data are compiled from measurements of many processes including thin strip casting, thin slab casting, and conventional billet and slab casting, much of it by Brimacombe [8]. Note that most of the data fall on roughly the same curve, despite the differences between the processes. Figure 5.2 shows that the average heat flux removed while the shell is in the mold correlates well with time without any extra gap formed between the mold and the shell. Based on these measurements, the following empirical formula is used to describe the average heat flux, $\bar{q}(MWm^{-2})$, as a function of contact time in the mold, $t_e(s)$.

$$\bar{q}(MWm^{-2}) = 4.05t_e^{-0.33} \tag{5.2}$$

This average heat flux curve is then generalized for any continuous casting process. The instantaneous heat flux, $q(MWm^{-2})$, is obtained by multiplying Equation 5.2 by $t_e(s)$ and then differentiating with respect to time. The function is truncated at short times to give:

$$q = \begin{cases} 12.4 & t \le 0.01 sec. \\ 2.71t(sec.)^{-0.33} & t > 0.01 sec. \end{cases}$$
(5.3)
By relating the time below the meniscus, t, to the casting speed, this instantaneous heat flux is transformed into a function of distance below the meniscus. Examples are shown in Figure 5.3 for four different cases with total heat extracted by a 1100mm long mold.

5.2 Materials Detail

Four steel grades are considered in this work: 0.003%C, 0.044%C, 0.1%C and 0.44%C carbon steels, which also contain 1.52%Mn, 0.34%Si, 0.015%S and 0.012%P. The solidus and liquidus temperatures, given in Table 5.1, are based on the non-equilibrium calculations of Won *et. al.* [167]. A critical strain criterion described in Section 2.2.2 is used to define failure of the shell. The damage strain described in Section 4.8 simplifies to the total strain for the thin slice domain because the total strain along the y direction shown in Figure 5.1 is perpendicular to the primary dendrite arms, which are along the x direction, and the same as the total strain across the brittle temperature range. The critical strains shown in Table 5.1 are calculated by Equation 2.1. The strain rate is taken just below the mold exit which is typically the highest strain rate during all the time below mold exit. This gives the smallest critical strain for a case and generates conservative fracture predictions. The critical strains decrease as the carbon content of of steel increases. This is because higher carbon steel has larger brittle temperature range.

5.3 Typical Results

Parametric studies are conducted with CON2D to investigate temperature, stress, and critical shell growth for total heat extracted by mold from 1.0 to $70MJm^{-2}$, section sizes from 50 to 400mm, working mold lengths from 300 to 1100mm and four different steel grades. Results for two typical simulations are shown in Figures 5.4 and 5.5 for 0.044% C steel cast in a 200mm square bloom mold with 700mm working mold length (800mm total length) with the total heat of $65.5MJm^{-2}$ and $7.4MJm^{-2}$ extracted by mold. The $65.5MJm^{-2}$ case is a normal amount of heat removed by mold in practice, while the $7.4MJm^{-2}$ case generates the critical shell thickness for this steel and mold. Figure 5.4 shows the surface temperature, shell thickness, inelastic strain rate and total strain histories for these two cases. Figures 5.5 show the temperature and stress distributions through the solidifying shell just below mold exit.

The surface temperature drops sharply just below the meniscus and then reheats. This is due to the very high heat flux expected at the beginning of solidification. Reducing the total heat removed by the mold generates a hotter and thinner shell at mold exit. As the strand moves below the mold, ferrostatic pressure starts to exert a load on the inside of the shell. At high heat removal case $(65.5MJm^{-2})$, the shell is thick enough to withstand this pressure so the inelastic strain rate due to creep is very small (less than $0.01\% sec^{-1}$). Thus, the total strain is dominated by the thermal shrinkage of the strand so decreases with distance below the mold.

For the $7.4MJm^{-2}$ heat removal case (generates critical shell thickness at mold exit), however, the thin and hot shell creeps rapidly under the ferrostatic pressure. This generates high inelastic strain rates, which reach a maximum of almost $10\% sec^{-1}$ just below mold exit. The inelastic strain rate continuously drops with distance below mold exit because the increase in shell thickness is much more important than the increase in ferrostatic pressure. The result is a rapid increase in tensile strain below mold exit, which reaches over 4.5% for this case. If the total strain reaches the critical fracture strain, (Table 5.1), the shell is assumed to have failed. Thus, the total strain saturates about 500mm below the mold exit for this case. In general, the most likely time for failure is in the first few seconds below mold exit, which corresponds to the time when many breakouts occur in practice.

Figures 5.5a and b show the temperature and stress profiles through the thickness of the solidifying shell for the two heat flux cases, respectively. Temperature increases almost linearly from the surface temperature (left) to the liquid (right). Naturally, there is no stress in the liquid and there should be virtually no stress in the mushy zone. It is significant to note that there is very little stress generated in the delta-ferrite portion of the solid shell. As the temperature drops, stress builds up in the cooler parts of the shell and reach a maximum at the shell surface. The colder austenite portion of the shell thus carries most of the stress.

5.4 Critical Shell Thickness

The results in the previous section showed that plastic strain due to creep will increase greatly just below the mold exit, if the shell is too hot and thin. The rate of creep strain accumulation decreases as the shell thickens. For each simulation in this study, this accumulation of strain is continued until the plastic strain rate dropped off to below $0.1\% sec^{-1}$. If the total strain at that moment reached the failure strain criterion measured for that steel (Table 5.1), then the shell is assumed to fail, as a longitudinal crack or breakout. The shell thickness at that time defines a critical shell thickness because the conditions which produce thicker shells never fail. In this work, the critical shell thickness is found for different steel grades, superheats, section sizes and mold lengths by decreasing the total heat removed by mold until the failure criterion is reached. The effects of each of these variables are shown in Figures 5.7 ~ 5.10.

Figure 5.7 shows the critical shell thickness for steels with different carbon contents cast under similar conditions. It is interesting that the critical shell thickness is nearly 3mm for all 4 grades, with the peritectic 0.1%C steel being slightly less. This indicates that the peritectic steel is actually slightly stronger and more crack resistant than the other steels. The fact that this steel is more crack prone in practice is thus due solely to its greater tendency to have shell surface nonuniformities that cause the local heat flux to be too small, leading to a local thinner shell. One of the factors generating nonuniform shell is the oscillation mark due to mold shaken whose purpose is to prevent mold sticking. Figure 5.6 shows the oscillation mark depth for steels with different carbon contents [9,176–180]. The peritectic 0.1%C steel has much deeper oscillation marks than other carbon steels. Thus, this steel grade thereby has a greater chance of having a local thin spot less than the critical thickness. Figure 5.7 also shows that the makeup of the shell changes greatly with steel grade. As the carbon content increases, the solid portion of the shell decreases. The shell also becomes stronger, however, because the austenite fraction increases. A much thicker δ -ferrite shell is needed to support the same load. On the other hand, the mushy zone becomes thicker as the carbon content increases with the wider freezing range. The net result is a critical shell that has about the same thickness, and requires about the same amount of heat removal to produce, for all of the grades.

Increasing superheat leads to a hotter and thinner solidifying shell, for a given heat removal. Consequently, the amount of heat needed to produce the critical shell thickness decreases. The critical shell thickness increases only slightly, however, owing to the hotter surface temperature. This slight effect of superheat is shown in Figure 5.8.

Increasing the section size causes the critical shell thickness increase, as shown in Figure 5.9. This is because a thicker shell is needed to withstand the larger ferrostatic load.

Shortening the mold length causes the critical shell thickness to increase, as shown in Figure 5.10. This is because the contact time is shorter, so the shell is hotter and weaker for a given thickness. Thus, a thicker shell is needed to get sufficient strength.

5.5 Critical Average Heat Flux in Mold

Decreasing the total heat removed by the mold results in hotter, thinner shells, which experience increased creep strain. This is seen in Figure 5.11, which shows the total strain (when inelastic strain rate drops to $0.1\% s^{-1}$) as a function of the average heat flux in mold for the 0.044% C steel. The strain which exceeds the critical fracture strain (4.5% for this steel) defines both the critical average heat flux in mold and the corresponding critical shell thickness, which is discussed in the previous section. The effect of steel grade, section size, and working mold length on critical casting speed are shown in Figure 5.12.

The effect of steel grade on critical average heat flux is shown in Figure 5.12a. The trends correspond naturally with the effect of grade on critical shell thickness. The thinnest critical shell, for 0.1%C steel, can tolerate the lowest average heat flux in the mold. Figures 5.8 and 5.12a both show that increasing the carbon content makes the solid portion of the shell stronger.

Figure 5.12b shows that increasing the working mold length allows lower average heat flux to be tolerated. This is because the contact time increases and leads to a larger amount of total heat extracted by the mold, then, a thicker shell at the mold exit. However, increasing the mold length requires increased attention to mold taper and lubrication. In order to maintain good contact between the shell and the mold, and thereby maintain good heat transfer, the mold must be tapered to match the shrinkage of the steel. This task becomes more difficult with a longer mold, which requires a nonlinear taper. In addition, the longer mold allows more time for the temperatures to drop and the liquid flux in the gap to solidify. Friction against the solid flux generates much higher longitudinal stresses in the shell, which could restrict the critical casting speed.

Figure 5.12c, shows that increasing the section size should increase the critical average heat flux. This is due to the greater ferrostatic pressure, as discussed for Figure 5.9. However, the average heat flux increase is less than linear.

5.6 Implications

The average heat flux in the mold is directly related to the shell thickness at mold exit. For the same casting speed and the working mold length, the higher is the average heat flux, the thicker and stronger is the shell thickness at the mold exit. However, as indicated at the beginning of this chapter, many phenomena influence the average heat flux in the mold. Among them, casting speed and the effective depth of oscillation marks are discussed here.

5.6.1 Casting Speed

Figure 5.2 indicates that increasing casting speed shortens the dwell time of the strand which increases the average heat flux, but lowers the total heat removed in the mold. The critical casting speed as a function of the steel carbon content, working mold length, and the section size are obtained from the critical average heat flux (Figure 5.12) and shown in Figure 5.13.

The effect of steel grade on critical casting speed is shown in Figure 5.13a. The trends correspond naturally with the effect of grade on critical shell thickness. The thinnest critical shell, for 0.1%C steel, can tolerate a highest casting speed.

Figure 5.13b shows that increasing the working mold length allows higher casting speed to be tolerated. This is because the contact time increases and leads to a larger amount of total heat extracted by mold, then, a thicker shell at the mold exit.

Figure 5.13c, shows that increasing the section size should decrease the critical casting speed. This is due to the greater ferrostatic pressure force, as discussed for Figure 5.9. As the average heat flux increases, the critical casting speed decrease with section size is less than linear.

The predicted huge critical casting speed (between 10 and 20 m/nin) is not possible in practice because other phenomena, such as sub-mold bulging, will lead to cracks and even "breakouts" before this speed can be reached. Therefore, only the local high heat resistance is able to generate the critical shell thickness as thin as 3mm.

5.6.2 Depth of Oscillation Marks

Figure 5.14 indicates that increasing the effective depth of the oscillation marks linearly decreases the average heat flux in the mold. This is due to the oil filled in the oscillation mark space have higher heat resistance than that of the steel. Casting conditions of the cases in Figure 5.14 are shown in Table 5.2. The relation between the average heat flux, $\bar{q}(MWm^{-2})$ in the mold and the oscillation mark depths, $d_{osc}(mm)$, are fitted from the measurements of

the oscillation mark depths shown in Figure 5.14.

1

$$\bar{q} = \begin{cases} 2.1993 - 0.92219d_{osc} &, V = 2.2m/min\\ 2.4178 - 0.65279d_{osc} &, V = 3.4m/min \end{cases}$$
(5.4)

The critical oscillation mark depths at 2.2m/min casting speed, as a function of the steel carbon content, working mold length, and the section size are obtained from the critical average heat flux (Figure 5.14) and Equation 5.4, and shown in Figure 5.15. The trends correspond naturally with the effect of grade, working mold length and the section size on critical average heat flux as discussed in previous section. Note that the critical oscillation mark depths are very close for all different parameters investigated, which indicates the average heat flux in the mold is very sensitive to the variations of the oscillation mark depths.

Note that the critical casting speeds and the critical oscillation mark depths indicated in this work are much higher than the practical casting speeds [10] and the oscillation mark depths [9] reported from industry. This implies that neither the casting speed nor the oscillation mark depth could generate the critical shell thickness at the mold exit alone. Figure 5.14 shows that increasing casting speed will decrease the oscillation mark depth. Therefore, the combination of these two factors is not likely to generate the critical oscillation mark depth reported in this work. The critical oscillation mark depths could represent the critical gap between the shell and the mold resulting the critical shell thickness. The critical gap values are at the order of a couple of millimeters which are very unlikely to encounter at a practical caster under proper operation conditions. This suggests that other issues need to be investigated as the primary factors causing "breakouts".

5.7 Figures and Tables



Fig. 5.1: Slice model domain with finite element mesh and region of shell modeled



Fig. 5.2: Average heat flux with respect to contact time (A - [5], B - [6], C - [7], D - [8])



Fig. 5.3: Instantaneous heat flux with respect to distance below meniscus casting at 2.2m/min(Total heat is for a 1100mm mold)



Fig. 5.4: Typical thermal-mechanical histories at strand surface (0.044% C carbon steel cast in 200mm square, 800mm long mold at 1.0m/min)



Fig. 5.5: Temperature and stress distribution through the solidifying shell (0.044% C carbon steel cast in 200mm square, 800mm long mold at 1.0m/min)



Fig. 5.6: Oscillation mark depth for steels with different carbon content [9]



Fig. 5.7: Carbon content effect on critical shell thickness (200mm square bloom, 800mm mold)



Fig. 5.8: Super heat effect on critical shell thickness (0.044% C steel cast in 200mm square bloom, 800mm long mold)



Fig. 5.9: Section size effect on critical shell thickness (0.044%C steel cast in 800mm long mold)



Fig. 5.10: Working mold length effect on critical shell thickness (0.044% C steel cast in 200mm bloom)



Fig. 5.11: Effect of total heat removed by mold and section size on total strain $(0.044\% C \text{ steel} \text{ at } \dot{\epsilon} = 10^{-3} sec^{-1})$



Fig. 5.12: Heat flux extracted by mold casting at 2.2m/min - influencing factors



Fig. 5.13: Critical casting speed - influencing factors



Fig. 5.14: Heat flux in mold as a function of oscillation mark depth [9]



Fig. 5.15: Critical oscillation mark depths at 2.2m/min - influencing factors

| Steel Type | Liquidus (^{o}C) | Solidus (^{o}C) | $\Delta T_B (^{o}C)$ | $\dot{\epsilon} (\% s^{-1})$ | ϵ_c (%) |
|------------|----------------------|---------------------|----------------------|------------------------------|------------------|
| 0.003% C | 1524.7 | 1496.9 | 2.78 | 0.88 | 6.1 |
| 0.044% C | 1521.0 | 1481.7 | 3.93 | 0.97 | 4.5 |
| 0.1%C | 1516.0 | 1460.8 | 5.52 | 0.77 | 3.4 |
| 0.44% C | 1485.4 | 1369.0 | 11.64 | 0.52 | 1.8 |

Table 5.1: Solidus and liquidus temperatures and critical strain

Table 5.2: Casting conditions for practice shown in Figure 5.14 for 0.27%C steel casting

| Osc. Mark | Osc. Mark | Frequency | Stroke | Pitch | |
|--------------|------------------|-----------|----------|-------|-------|
| Depth (mm) | Width (mm) | (cpm) | (mm) | (mm) | |
| | V=2.2 and 3.4r | 2.2m/min | 3.4m/min | | |
| 0 | 0 | 30 | 2 | 1.89 | 1.22 |
| 0.1 | 2 | 6 | 4 | 9.44 | 6.11 |
| 0.2 | 4 | 3 | 8 | 18.89 | 12.22 |
| 0.4 | 8 | 1.5 | 12 | 37.78 | 24.44 |
| 0.5 | 10 | 1.5 | 12 | 37.78 | 24.44 |
| 0.65 | 13 | 1.5 | 12 | 37.78 | 24.44 |

Chapter 6. Billet Sub-Mold Bulging

Sub-mold bulging is an important factor influencing the initiation of various internal cracks as discussed in Chapter 1. Partially solidified steel shell is taken ferrostatic pressure from the liquid steel due to gravity and bulges out. This issue becomes more severe for billet casting due to its lack of sub-mold support rollers. Sub-mold bulging leads to tensile stress and inelastic strain near the solidification front around strand corner and intends to generate off-corner sub-surface cracks when the stress or strain is high enough [121].

CON2D is applied to simulate one quarter of a billet section to predict the evolution of its temperature, stress and strain of a 0.27%C plain carbon steel for various section sizes and working mold lengths. The casting speed is increased for each modelled case until the maximum damage strain exceeds the critical strain leading to hot tear cracks. The casting speed in which the hot tear cracks just initiate is the critical casting speed to avoid the hot tear cracks.

6.1 Modeling Domain

The modeling domain is a L-shaped region in one quarter of a transverse section from continuous casting steel billet assuming symmetrical temperature and stress distributions about the billet center lines, as shown in Figure 4.1. Figure 4.2 shows the mesh of the 3node triangle elements used for heat transfer analysis and 6-node mesh of triangle elements for stress analysis, respectively.

This domain includes the entire solid shell in the upper portion of the caster, but ignores some of the liquid near the billet center to save on computation requirements. Smaller size elements, 0.1mm, are used near the surface to produce more accurate thermal stress/strain prediction during the initial solidification period. Larger size elements, 1.0mm, are used near the center to reduce computational cost substantially, without sacrificing much accuracy. This choice is validated by comparing with an analytical solution discussed in section 4.10.

6.2 Heat Flux Profile

The instantaneous interfacial heat flux profile down the mold is usually found from thermocouple measurements in the mold. The profile is then integrated to find the average heat flux in the mold, which should match a global heat balance with the cooling water. In this work, the procedure is reversed to estimate the instantaneous heat flux profile. The average heat flux data points measured by several investigators [6, 10, 15, 181–183] and its fitted average heat flux curve, which is expressed by Equation 6.1, are shown in Figure 6.1. Slab caster data with mold flux is seen to be lower than billet cast means lubricated with oil. It represents the billet casting with oscillation marks between 0.2 and 0.6mm deep [9]

$$\bar{q}(MWm^{-2}) = 9.5579t(s)^{-0.504}$$
(6.1)

The instantaneous heat flux function of distance down the mold, which is needed in the model, is obtained by differentiating Equation 6.1. At short times, the instantaneous heat flux drops linearly with time, which is indicated by strip casting research [184, 185]. This assumption also avoids the unrealistic high instantaneous heat flux produced by differentiation. The instantaneous heat flux function is given in Equation 6.2 and heat flux curves for several casting speeds are plotted in Figure 6.2.

$$q(MWm^{-2}) = \begin{cases} 5 - 0.2444t(s) & t \le 1.0s \\ 4.7556t(s)^{-0.504} & t > 1.0s \end{cases}$$
(6.2)

The instantaneous heat flux is assumed to be uniform around the perimeter of the billet surface. This corresponds to the assumptions of ideal taper and perfect contact between the shell and mold. After the billet leaves the mold, its surface temperature is kept unchanged from its circumferential profile at mold exit. This eliminates the effect of spray cooling practice on sub-mold reheating or cooling cycling which leads to surface stress/strain variation and generates more cracks, then, slows down casting speed. This configuration and the ideal mold taper [186] lead to upper limit of the critical casting speed to avoid hot tear cracks. Fluid flow in the liquid pool may create non-uniform removal of the superheat [163]. The effect is minor when the pouring temperature is close to liquidus temperature and is ignored in this work, which treats superheat in the liquid with simple conduction.

6.3 Parametric Study and Computational Details

To investigate the maximum casting speeds under different mold lengths and section sizes, nine sets of simulations are performed for the 3 mold lengths and 3 section sizes shown in Table 6.1 for 0.27% plain carbon steel whose chemical compositions and the phase transformation temperatures are listed in Table 6.2.

For each section size and working mold length, simulations are performed with various casting speeds and evaluated using both hot tear failure criteria in discussed in section 2.2.2 and 1mm maximum sub-mold bulging criterion to determine whether the failure of the shell occurs. The damage strain is obtained by accumulating inelastic strain component along "hoop" direction of the solidifying shell. The "hoop" direction is defined along x-axis for the horizontal part and y-axis for the vertical part of the modeling domain in Figure 4.2. This direction is perpendicular to the primary dendrite arms. The case with 120mm section size and 700mm working mold length, which is highlighted in Table 6.1, is chosen as a base case to analyze since it is widely used at many casters. Mesh size continuously changes from 0.1mm to 1.4mm from slab surface to the center. Time step size stepwisely changes from 0.001*sec.* to 0.5*s*. Each simulation is divided into two parts, one within the mold and the other below the mold. It takes approximately 4 hours to complete a single simulation with around 4000 time steps on a dual Pentium III 933MHz CPU workstation with 1GB RAM running Windows 2000 Pro OS.

6.4 Typical Results

6.4.1 Heat Transfer Model Results

Figure 6.3 shows the shell thickness histories of the base case for 2.2m/min and 5.0m/min casting speed. The shorter dwell time in the mold leads to less total heat extracted. Thus, the shell thickness at the mold exit is thinner at higher casting speed.

Figure 6.4 shows the corresponding billet surface temperatures. Naturally, higher surface temperature is produced by higher casting speed, due to the shorter time at any given distance down the mold. However, the increase is not very large because of the higher heat flux produced at shorter times (high speed) as given in Figure 6.1. Figure 6.5 shows the surface temperature at mold exit which is assumed to stay unchanged below the mold exit. Surface temperature far from the corner is approximately constant due to one-dimensional heat transfer. Temperature drops toward the corner despite the constant heat flux profile around the perimeter. This is due to 2D heat transfer at the corner.

6.4.2 Stress Model Results

Figure 6.6 shows the distorted temperature contours at mold exit and 200mm below the mold exit for both casting speeds. It is observed that the thinner, hotter, and weaker shell bulges more at high casting speed under the ferrostatic pressure. Figure 6.10 quantifies the extent of surface displacements at mold exit and 200mm below mold exit for both casting speeds. This shows that bulging increases rapidly after a threshold has been crossed in either excessive temperature or insufficient shell thickness.

Figures 6.7 and 6.8 show hoop stress and total strain contours constructed from the stress results based on stress and strain in x direction at horizontal arm and the y direction at vertical arm. High values appear at the off-corner sub-surface region, due to a hinging effect that the ferrostatic pressure over the entire face exerts around the corner. This bends the shell around the corner and generates the high subsurface tensile stress at the weak solidification front in the off-corner subsurface location. This tensile stress increases at higher casting speed. There is no obvious high stress and strain region at the low casting speed. Surface hoop stress and total strain are compressive at mold exit and remain compressive at low casting speed. This indicates no possibility of surface cracking. However, tensile surface hoop stress and strain are generated below the mold at high speed in Figures 6.717d and 6.8d at face center due to excessive bulging. These tensile stress and strain might contribute towards surface longitudinal cracks.

Figures 6.11 and 6.12 show the evolution of the strains for the point at (6.7mm, 17.4mm), which is in the high strain region (off-corner subsurface), for the two casting speeds. Little plastic strain is developed when the billet exits the mold at normal casting speed, 2.2m/min. Substantial plastic strain is developed at higher casting speed, 5.0m/min. Moreover, much more inelastic strain, flow strain and plastic strain, is developed during the brittle temperature range, ΔT_B , between 90% and 99% of solid forms. Inelastic strain developed here could contribute to longitudinal hot tearing cracks at the off-corner subsurface location. The strain histories also indicate that most of the inelastic strain develops just below mold exit. As the billet moves farther below mold exit, the shell thickens and becomes strong enough to withstand the ferrostatic pressure, as the average temperature across the billet section drops.

Figure 6.13 shows contours of the out-of plane stress, (along z axis: casting speed direction), for this case at both casting speeds of 2.2m/min and 5.0m/min. High tensile z-stress is found at the corner region for both cases. This is due to over cooling from the 2D heat extraction there. The colder corner tries to shrink more than the off-corner and center regions. However, each x-y section through the long billet has to remain planar. Thus, the corner region is stretched by the off-corner region, while the off-corner region is squeezed by the corner region. As a consequence, axial tensile stress is developed at the corner region and compressive stress at the off-corner. This tensile stress might contribute to forming transverse corner surface cracks.

6.4.3 Failure Mechanism

The damage strain accumulated during the brittle temperature range could lead to hot tearing cracks because the thick dendrites in this temperature prevent the surrounding liquid from compensating the solid expansion. Figure 6.14 shows the contours of damage strain accumulated during the brittle temperature range, ΔT_B , for the 120mm section size and 700mm working mold length with two casting speeds of 2.2m/min and 5.0m/min. The highest values of damage strain appear at the off-corner sub-surface region along the "hoop" direction which is perpendicular to the growth direction of the primary dendrite arms. This location matches the position of the crack in Figure 6.9. The maximum value of the damage strain and the number of nodes which exceed the corresponding critical strain for all the casting speeds simulated for this case (120mm section and 700mm working mold length) are also listed in Table 6.3. Moreover, significantly higher values (1.5% and 1.7%) are found for the higher casting speed cases (5.0m/min and 6.0m/min). At 5.0m/min casting speed, the damage strain in the hoop direction exceeds the damage threshold (0.49%) calculated by Equation 2.1 at 16 nodes, all located near the off-corner subsurface region. This is caused by the hinging mechanism around the corner. Only 1 node exceeds the threshold of 0.9%at 2.2m/min casting speed. Note that the strain has oscillation peaks due to convergence difficulty. So, no failure is considered if there are less than 5 nodes exceeding the threshold. Therefore, the critical casting speed below which no hot tear crack initiates is 5m/min.

Figure 6.15 shows damage strain contours in z direction at both speeds (2.2m/min) and 5.0m/min). The damage strain is very small (~ 0.075%) for all nodes. No nodes fail in the axial direction even at high casting speed. Therefore, it is the longitudinal off-corner subsurface hot tear cracks, and not transverse surface corner cracks that limit the casting speed.

6.4.4 Critical Casting Speed

Using the damage criterion described by Equation 2.1, a casting speed limit to avoid crack initiation can be obtained by running many cases with various casting speeds. The minimum speed having failed nodes is the critical speed limit for that section size, mold length and steel grade. For the base case, with 120mm section size and 800mm mold length, the critical casting speed is close to 5.0m/min. This roughly agrees with the experimental findings [187]. The practical casting speed limit varies from 2m/min of a 200mm square section to 3m/minof a 130mm section with 800mm mold length. From the previous discussion, higher casting speed leads to higher inelastic strain at off-corner sub-surface region as well as larger bulging, as indicated by Figure 6.16. It indicates that sub-mold bulging will eventually stop increasing due to the shell growth.

The maximum bulging is plotted versus casting speed in Figure 6.17. This reveals how the maximum bulging increases with casting speed. The maximum bulging increases sharply as casting speed increases near the critical casting speed indicated by hot tear criterion. This sharp threshold suggests that the critical casting speed might not be particularly sensitive to steel grade.

Figure 6.17 could be used to determine casting speed limit under any specific maximum bulging criterion. A maximum bulging of 4mm to 10mm corresponds to avoid hot tear off-corner sub-surface cracks. The critical speeds to avoid cracks, thus, are higher than the critical speeds to satisfy the 1mm maximum bulging criterion, given the same section size and mold length.

6.4.5 Effect of Section Size and Mold Length

Figures 6.19 and 6.20 show the critical speed for different section sizes and working mold lengths, based on the hot tear criterion and the 1mm maximum bulging criterion, respectively. The working mold length is shortened by a half of the section size, from small hollowed symbols to small solid symbols as shown in Figure 6.18, to take into account the

axial support of the billet from mold bottom due to cantilever effect. This is missing in this model because the moving slice deforms without much interaction among its neighbors. Then, corrected data is scaled back, larger solid symbols as shown in Figure 6.18, to the working mold lengths being modelled, which are 500mm, 700mm and 1000mm.

The critical casting speed increases as the working mold length increases for a given section size. For example, the critical casting speed based on the cracking criterion increases from 4.2m/min to 6.4m/min as the working mold length increases from 500mm to 1000mmfor a $120mm \times 120mm$ square billet. This is due to colder and thicker shell at mold exit for the longer dwell time in the mold. The critical speed decreases as the section size increases in a given mold length. For example, the critical casting speed based on the cracking criterion decreases from 5m/min to 2m/min as the section size increases from 120mm to 250mmfor a 800mm mold. It is very sensitive to the mold section size because the larger surface subjected to ferrostatic pressure provides a lever arm for much bending around the corner.

The CON2D predicted casting speed limits based on hot-tear criterion and 1mm maximum bulging criterion are compared to measured casting speeds from typical industrial practices [10]. CON2D predictions are generally more conservative due to the perfect mold operating condition assumption. Ideal mold taper which prevent any gap between the mold wall and the shell surface can hardly be implemented in practice. Therefore, corners of billets are often hotter and weaker then those predicted by CON2D. The friction between the mold wall and shell surface will also lower the real casting speed limits.

6.5 Implications

Productivity is always a consideration interest for caster designers and operators. The critical casting speed plots developed in this work are useful guidelines for casting engineers in choosing safe casting speeds. Table 6.4 predicts the corresponding productivity limits, based on both the off-corner longitudinal crack criterion and 1mm maximum bulging criterion.

The intuitive productivity benefit from large section size is almost offset by the lower casting speed limits to avoid excessive bulging or off-corner cracks. Casting at the desired cross section size to minimize rolling cost will not lose much productivity. Longer mold length increases the productivity limits. This is because the thicker, colder shell allows higher casting speed before bulging below the mold becomes excessive. Based on this finding, extra sub-mold support, such as properly aligned foot rolls, should also allow increasing productivity. The latter approach avoids the problems associated with longer molds, as surface temperature can be easily controlled by sprays and the shorter mold is less sensitive to mold taper problems.



Fig. 6.1: Measured average heat flux and fitted average heat flux curve



Fig. 6.2: Instantaneous heat flux curve



Fig. 6.3: Shell thickness history (Section size: 120mm, working mold length: 700mm)



Fig. 6.4: Surface temperatures history (Section size: 120mm, working mold length: 700mm)



Fig. 6.5: Surface temperature at mold exit and below (Section size: 120mm, working mold length: 700mm)



(b) 2.2m/min at 200mm below mold exit (d) 5.0m/min at 200mm below mold exit

Fig. 6.6: Distorted temperature contour at mold exit (Section size: 120mm, working mold length: 700mm)



(b) 2.2m/min at 200mm below mold exit
(d) 5.0m/min at 200mm below mold exit
Fig. 6.7: Hoop stress contours (Section size: 120mm, working mold length: 700mm)



(b) 2.2m/min at 200mm below mold exit (d) 5.0m/min at 200mm below mold exit Fig. 6.8: Hoop total strain contours (Section size: 120mm, working mold length: 700mm)



Fig. 6.9: Continuous-cast billet section after breakout showing off-corner subsurface crack



Fig. 6.10: Surface displacements at mold exit and 200mm below (Section size: 120mm, working mold length: 700mm)



Fig. 6.11: Histories of strains at (6.7mm, 17.4mm) (Section size: 120mm, working mold length: 700mm, Speed: 2.2m/min)



Fig. 6.12: Histories of strains at (6.7mm, 17.4mm) (Section size: 120mm, working mold length: 700mm, speed: 5.0m/min)



Fig. 6.13: Stress along casting direction (Z direction) at mold exit (Section size: 120mm, working mold length: 700mm)


(a) 2.2m/min at 850mm mold exit

(b) 5.0m/min at 1920mm below mold exit

Fig. 6.14: Hoop damage strain (Section size: 120mm, working mold length: 700mm)



Fig. 6.15: Z damage strain at mold exit (Section size: 120mm, working mold length: 700mm)



Fig. 6.16: Displacement histories at surface center (Section size: 120mm, working mold length: 700mm)



Fig. 6.17: Maximum bulging vs. casting speeds



Fig. 6.18: CON2D predicted critical casting speeds and corrected critical speeds accounted partial mold end support



Fig. 6.19: Comparison of the critical speeds based on hot-tear criterion and typical plant practice [10]



Fig. 6.20: Comparison of the critical speeds based on 1mm maximum bulging criterion and typical plant practice [10]

| Billet section size $(mm \times mm)$ | $120 \times 120, 175 \times 175, 250 \times 250$ |
|---|--|
| Working mold length (mm) | 500, 700, 1000 |
| Total mold length (mm) | 600, 800, 1100 |
| Taper $(\%m)$ | Ideal taper (on both face) |
| Time to turn on ferrostatic pressure $(sec.)$ | 0.3 |
| Mesh size $(mm \times mm)$ | $0.1 \times 0.1 \sim 1.4 \times 1.0$ |
| Number of nodes (varies with section size) | 7381, 10797, 15433 |
| Number of elements (varies with section size) | 7200, 10560, 15120 |
| Time step size $(sec.)$ | $0.001 \sim 0.5$ |
| Pouring temperature (^{o}C) | 1540.0 |

Table 6.1: Parametric study conditions

Table 6.2: Steel compositions and important transforming temperatures

| Steel composition $(wt\%)$ | 0.27C, 1.52Mn, 0.34Si, 0.015S, 0.012P |
|---|---------------------------------------|
| Liquidus temperature (^{o}C) | 1500.72 |
| 70% Solid temperature (°C) | 1477.02 |
| 90% Solid temperature (°C) | 1459.90 |
| Solidus temperature (^{o}C) | 1411.79 |
| Austenite $\rightarrow \alpha$ -ferrite starting temperature (°C) | 781.36 |
| Eutectoid temperature (^{o}C) | 711.22 |

Table 6.3: Critical strains (%)

| Casting speed (m/min) | 2.2 | 3.0 | 4.0 | 4.6 | 4.8 | 5.0 | 6.0 |
|------------------------------|------|-----|------|------|------|------|------|
| Critical strain (%) | 0.91 | 0.9 | 0.9 | 0.66 | 0.59 | 0.49 | 0.52 |
| maximum damage strain $(\%)$ | 0.94 | 0.8 | 0.92 | 0.97 | 1.05 | 1.50 | 1.76 |
| Number of failed notes | 1 | 0 | 1 | 2 | 4 | 16 | 26 |

Table 6.4: Productivity limits $(tonnemin^{-1})$

| Mold length (mm) | Longitudinal off-corner | | | 1mm maximum | | | |
|---------------------|-------------------------|------------------|------------------|------------------|------------------|------------------|--|
| | Crack criterion | | | Bu | ılging criteri | on | |
| Section size (mm) | 120×120 | 175×175 | 250×250 | 120×120 | 175×175 | 250×250 | |
| 600 | 0.4 | 0.7 | 0.7 | 0.4 | 0.5 | 0.4 | |
| 800 | 0.6 | 0.9 | 0.9 | 0.5 | 0.6 | 0.5 | |
| 1100 | 0.7 | 1.0 | 1.2 | 0.6 | 0.8 | 0.7 | |

Chapter 7. Ideal Taper Prediction

Mold taper is an important control parameter in the continuous casting of steel billets. Properly tapered mold walls compensate for shrinkage of the solidifying strand to maintain good contact and heat transfer between the mold wall and shell surface without exerting extra force on the hot and weak shell. The amount of taper needed varies with steel composition and casting conditions, such as mold length, casting speed, and type of lubrication. Inadequate mold taper leaves an air gap between the mold wall and shell surface which leads to a hotter and thinner shell within the mold which partly relates to criterion 4. Ferrostatic pressure from the liquid core will bulge the weak shell within and out of the mold and even break out the shell in extreme situations. Excessive taper exerts extra load on the solidifying shell and increases dragging friction which relates to criterion 2. Transverse cracks, shell buckling or even shell jamming and breakouts may occur. Past efforts conducted to assist mold taper prediction includes mathematical models to calculate thermal shrinkage of the steel billet [51, 70, 71] and thermal distortion of the mold [67, 70, 175, 188]. These previous investigations assume optimal taper should match the shell shrinkage, presuming this should produce good heat transfer across the interfacial layer between mold wall and billet surface at the face center along the mold axial direction. Corner effects have received little attention.

Traditionally, it is assumed that optimal taper should exactly match shell shrinkage everywhere around the mold perimeter. However, corner effects are complex and providing proper taper to match corner shrinkage is very important. To understand the thermalmechanical behavior of the billet especially at corner, three different mold configurations have been simulated under two casting speeds, 2.2m/min and 4.4m/min, which are within the normal industrial operation range. The first configuration is taken from a plant trial conducted at POSCO, Pohang works, South Korea [41]. A single linear taper of $0.75\% m^{-1}$ is used during this trial. The second configuration assumes perfect contact between mold wall and shell surface around the billet perimeter. This implies uniform heat flux around the mold perimeter. This is an idealized condition that requires a complex mold wall surface following the shell shrinkage everywhere from the meniscus to the mold exit. The third configuration is a different idealized mold wall shape, which produces uniform surface temperature around the billet perimeter. The actual shape is unknown before the simulation is conducted. It can be extracted by backward calculation according to the heat flux function around the billet surface and air gap properties.

Although these mold configurations would be very difficult to implement in practice, the conditions are easy to achieve in the model. They are simply three different thermal boundary conditions applied at the billet surface:

- 1. Heat transfer resistor model between shell surface and mold wall which requires fully coupled thermal-stress simulation.
- 2. Uniform heat flux around the billet perimeter as a function of casting time.
- Uniform surface temperature around the billet parameter as a function of casting time. Each is discussed in turn.

7.1 Heat Transfer Resistor Model ($0.75\%m^{-1}$ Taper)

The first configuration simulates a realistic operating practice of flat mold walls with a fixed taper of $0.75\% m^{-1}$. Figure 4.3 shows the heat transfer resistor model assumed between the mold wall and the shell surface. The values of the parameters are given in Table 4.1. The values of cooling water temperature and its heat transfer coefficient vary from meniscus to mold exit. The actual profiles are taken from a more advanced heat transfer model, CON1D [2]. The contact resistance differs from its physical value between steel and copper because it also includes the effect of oscillation marks is included. The heat extraction rate is mainly determined by the gap in the interfacial layer, which further depends on the instantaneous mold wall distortion and the shrinkage of the shell. Mold distortion from Equation 4.39 is given in Figure 7.1.

The shrinkage of the shell is taken from the mechanical analysis. Since the temperature and stress/strain distributions depended on each other and are unknown in prior, a fully coupled simulation procedure as previously given in Figure 4.4 is needed. At each time step, the gap size from the previous time step is used to estimate the heat transfer rate and the heat transfer Equations are solved. Then, the mechanical model is solved based on the new temperature distribution to give out a new gap. The two-step procedure is repeated until the gap sizes from two successive iterations are close enough.

7.2 Uniform Heat Flux Around Mold Perimeter Model

The instantaneous interfacial heat flux profile down the mold in this case is obtained by differentiating the average heat flux profile, fitted from average heat flux data points measured by many investigators [6, 10, 15, 181–183]. In addition, the instantaneous heat flux function is compared with instantaneous heat flux measurements by Samarasekera and coworkers [189]. Equations 7.1 and 7.2 show the fitted average and instantaneous heat flux functions. Figures 7.2 and 7.3 compare the average and instantaneous heat flux curve against the measurements.

$$\bar{q}(MWm^{-2}) = 13t(s)^{-1}[(t(sec.) + 1)^{0.5} - 1]$$
(7.1)

$$q(MWm^{-2}) = 6.5(t(s) + 1)^{-0.5}$$
(7.2)

7.3 Uniform Surface Temperature Around Mold Perimeter Model

The third mold configuration fixes the surface temperature to be uniform around the mold perimeter, and is shown in Figure 7.4. This profile is identical to the surface temperature profile generated down the face center while the heat flux function (Equation 7.2) is applied.

7.4 Secondary Cooling Pattern

After the billet exits the mold, it enters the secondary cooling region. A heat convection coefficient function suggested by Nozaki [16] is adopted in this work. The secondary cooling rate in this work is designed to minimize the sudden surface temperature change at the face center when the billet leaves the mold. Figure 7.5 shows the heat transfer coefficient profile for both casting speeds.

7.5 Billet Behavior For Different Mold Configurations

CON2D is applied to predict thermal-mechanical behavior of billets cast under the 3 different mold configurations described previously. The optimal taper strategy will be chosen based on avoiding both in-mold and below-mold cracks as well as excessive bulging. The simulation results are evaluated according to the effects on the shell growth, sub-mold bulging, and transverse corner cracks as well as longitudinal off-corner sub-surface cracks.

7.5.1 Surface Temperature and Shell Growth

Figure 7.6 shows the temperature contours at the mold exit for the three types of mold configurations. The liquidus at $1500.72^{\circ}C$ and solidus at $1411.79^{\circ}C$ isothermals mark the shell growth at mold exit.

Both the mold configurations with uniform heat flux and uniform surface temperature around the mold perimeter produce a thicker shell near the corner relative to the shell near the face center. This is due to 2D cooling. The shell thicknesses at billet face center for the mold with $0.75\% m^{-1}$ linear taper in Figures 7.6a and 7.6b are much thinner than those with the mold providing the prescribed surface heat flux in Figures 7.6c and 7.612d as well as the uniform surface temperature in Figures 7.6e and 7.6f. This indicates that $0.75\% m^{-1}$ is much less than ideal taper at face center. This practical mold configuration also leads to a hot spot at the off-corner region at 2.2m/min speed in Figure 7.6a. This indicates that more taper is needed both in the top region of the mold and near the corners to avoid the hot spots.

Figure 7.7 compares the surface temperature histories starting from the meniscus at the billet corner for the three different mold configurations described above. The traditionally believed optimal taper, which perfectly follows the shell shrinkage everywhere, and which corresponds to the uniform heat flux configuration, produces an extremely cold corner in the mold. When the billet leaves the mold, there is nearly $200^{\circ}C$ reheating near the corner despite the spray zone design to minimize surface temperature change at the billet face center. The corner cools faster than for the other two mold configurations due to 2D heat convection in the secondary cooling zone. Previous investigations of internal cracks [23,25] suggest that reheating should be avoided to prevent internal cracks. Thus, an extremely cold corner is not favorable, which means that the traditional strategy for optimal taper design is not optimal near the corner.

7.5.2 Sub-Mold Bulging and Longitudinal Off-corner Sub-Surface Cracks

As the billet leaves the mold, ferrostatic pressure from the liquid core due to gravity is totally supported by the solidifying shell and produces sub-mold bulging. The amount of bulging is determined by the strength of the shell. A hot and thin shell having low strength will bulge more. The more severe creep at higher temperature makes the shell bulge even further. Figure 7.8 shows the stress component along the shell surface with distorted shell for the billet casting in the mold with $0.75\%m^{-1}$ linear taper at 100mm below the mold exit. The amount of bulging is small while casting at 2.2m/min (< 0.5mm), but increases nearly 8 times when the casting speed is doubled. The ferrostatic load bends the billet shell around the corner generating tensile stress along the solidifying front. This tensile stress is perpendicular to the growth direction of the dendrite arms and may lead to sub-surface cracks beneath the surface region about $10 \sim 15mm$ from the corner. Recent experiments of steel strength near its melting temperature [110] indicates that the strength of plain carbon steel is around 10MPa at $1300^{\circ}C$ which is the same as the maximum tensile stress value in Figure 7.8b. This implies that fracture is highly possible around the sub-surface off-corner region in Figure 7.8b. Figure 7.9 shows the damage strain component along the solidification front which leads to hot tear cracks according to Equation 2.1. The critical strain is calculated as $0.6\% \sim 1\%$ from Equation 2.1. The damage strain at two off-corner regions near the solidification front exceeds the critical strain by over 60% when the casting speed is doubled to 4.4m/min. This provides further evidence that hot tear cracks initiate for this condition. Therefore, a mold design with more taper to cool the corner is needed to avoid excessive bulging and longitudinal sub-surface off-corner cracks below the mold.

7.5.3 Transverse Corner Cracks

Although a very cold corner may prevent bulging and off-corner cracks, it has its own shortcomings. A very cold corner in the mold will suffer reheating in the secondary cooling zone. Previous research by Grill [23] and Sorimachi [25] already indicated that reheating should be avoided to prevent sub-surface cracks. Figure 7.10 shows the contours of the stress component along axial direction for the billet with the uniform heat flux around the perimeter at 100mm below the mold exit. The corner is reheated from around $400^{\circ}C$ to $600^{\circ}C$ at this distance. The totally solidified steel near the surface tries to expand under reheating. This exerts tensile stress at the sub-surface region. Figure 7.10 shows high tensile stresses at the corner sub-surface region. This high tensile stress region is closer to the solidification front at higher casting speed. Although the damage strain is not over the critical value for these speeds, it is believed that transverse sub-surface corner cracks would initiate when the casting speed is increased further.

Figure 7.11 shows contours of the stress component along the billet axial direction for the billet with the uniform heat flux around the perimeter at two different locations (100mm for 2.2m/min and 200mm for 4.4m/min) below meniscus. Tensile stress up to 30MPa near the corner surface is indicated. This is because the corner surface cools faster than its subsurface layer. Transverse corner surface cracks are easily initiated under this stress state if the friction between the mold and the billet is considered, or if any other problems existed such as mold misalignment or stress concentration at deep oscillation marks. Thus, very cold corners should be avoided to prevent transverse corner surface cracks and sub-surface cracks.

7.6 Optimal Taper Profiles Near Billet Corner

It has been found that an optimal mold taper should avoid both very cold or very hot billet corners in order to avoid cracks or excessive bulging. Therefore, the optimal taper should have the following features:

- 1. It should be large enough to follow the shrinkage of the billet around the face center to avoid gap formation.
- 2. It should allow some amount of gap between the billet surface and the mold wall to offset the over cooling caused by 2D heat transfer near the billet corner so that the surface temperature of the billet is uniform around the perimeter.

This is consistent with industrial practice that uses less taper near the corner [69]. Since some gap is needed near the billet corner, the optimal taper could not be determined by only analyzing billet shrinkage. Conditions of the heat flux profile near the corner as well as the heat resistance across the gap are also needed. This makes the optimal taper prediction much more complex. Figure 7.12 shows the heat flux at the shell surface and the gap size near the corner at mold exit that are needed to achieve the uniform surface temperature around the mold perimeter. The heat flux is quite uniform away from the billet corner with its value described by Equation 7.2. The heat flux drops near the corner to compensate the 2D heat transfer. The mold should be designed to leave a gap on the order of 0.1mmbetween the billet and the mold from 13mm from the corner in order to reduce the heat transfer. The optimal gap is only predicted up to 4mm from the corner since the round corners of real molds are not modelled in this work. The dashed line indicates the ideal mold wall position predicted by the CON2D model with a numerically simple 1D slice domain. This 1D prediction is surprisingly accurate at the corner as it leaves a gap up to 0.15mm even though it does not consider the corner effect totally.

Figure 7.13 shows the shrinkage of the billet under different assumptions of mold operation compared with the $0.75\%m^{-1}$ linear taper case. The billet shrinkage profile with the uniform surface temperature compares closely to the ideal taper prediction of the 1D thermal stress model. Considering that the optimal taper should be less than the billet shrinkage to allow some gap near the billet corner, the ideal taper prediction of the 1D slice model is a reasonable estimation method.

7.7 Optimal Taper Profiles

The 1-D slice model of CON2D has been adopted to investigate the effects of casting speed and heat flux on optimal taper profile including the effects of the mold distortion. Details of the slice model are discussed in section 5. The shrinkage profiles of the billet are given in Figure 7.14 up to 1000mm assuming the average heat flux between the mold and the billet is only a function of dwell time as given in Equation 7.1. It can be observed that the instantaneous taper is not linear. Larger taper is needed near the meniscus and for shorter molds. This is mainly due to the instantaneous heat flux profile. Heat flux is high near the meniscus and drops monotonically thereafter. Multifold linear taper or parabolic taper is recommended to prevent a general gap between the mold and billet surfaces near the meniscus. As the casting speed increases, the amount of mold taper should be reduced accordingly, due to less dwell time, the billet stays in the mold shorter which decreases the total heat extracted.

Figure 7.15 shows the shrinkage of the billet at 1000mm below meniscus as a function of casting speed. The high heat flux curve corresponds to the heat flux profile fitted by Wolf [182] for billet casters, while the lower one corresponds to the heat flux profile fitted by author in section 6. These two profiles enclose most of the published average heat flux measurements for billet casters [182, 183]. Smaller taper is needed when the average heat flux in the mold is lower. It is also consistent to Figure 7.14 that mold taper should be reduced as the casting speed increases.

Figure 7.16 shows the shrinkage of the billet at mold exit as a function of the total heat extracted from the mold for different casting speeds and mold lengths. At each casting speed, the shrinkages are measured for different working mold lengths, 50mm, 200mm, 500mm, 700mm and 1000mm. It is observed that the shrinkage depends on the total heat extracted by the mold only. The profiles for different casting speeds collapse into one profile, which indicates that the total heat removed in the mold is a more fundamental parameter controlling the amount of taper needed at the mold exit than either casting speed, or mold length. This important finding is true in general if the shape of the instantaneous heat flux profile stays the same for all different casting speeds.

Figure 7.17 shows the maximum mold distortion at mold exit as a function of the average heat flux for different casting speeds and working mold lengths, based on Equation 7.1. The profiles for different casting speeds again collapse to a single curve. This indicates the average heat flux in the mold is the fundamental parameter controlling the mold distortion. Mold distortion naturally increases with the average heat flux, owing to the higher mold temperature. This mold distortion should be taken into account when designing mold taper.

7.8 Figures and Tables



Fig. 7.1: Mold distortion for 2-D simulation



Fig. 7.2: Measured average heat flux and fitted functions



Fig. 7.3: Instantaneous heat flux curve



Fig. 7.4: Uniform surface temperature



Fig. 7.5: Heat transfer coefficient in spray zone



Fig. 7.6: Temperature contours at the mold exit 181



Fig. 7.7: Surface temperature histories casting at 2.2m/min for three mold configurations



Fig. 7.8: Stress contours at 100mm below mold exit casting in the $0.75\%m^{-1}$ linear taper mold (inadequate taper)



Fig. 7.9: Damage strain contours at 100mm below mold exit casting in the $0.75\%m^{-1}$ linear taper mold (inadequate taper)



Fig. 7.10: Axial stress contours at 100mm below mold exit casting in the mold with too much taper



(a) 2.2m/min, 100mm below meniscus (b) 4.4m/min, 200mm below meniscus Fig. 7.11: Axial stress contours in the mold with too much taper



Fig. 7.12: Shell shrinkage, heat flux and gap at the mold exit casting at 2.2m/min with the ideal mold taper (uniform surface temperature)



Fig. 7.13: Optimal taper prediction



Fig. 7.14: Optimal taper profiles predicted by slice model



Fig. 7.15: Shrinkage at 1000mm



Fig. 7.16: Shrinkage at mold exit vs. total heat extracted by mold



Fig. 7.17: Maximum mold distortion vs. average heat flux

Chapter 8. Summary

A finite element thermal mechanical model, CON2D, is improved and then applied to investigate the minimum heat flux and shell thickness for continuous casting of steel due to strength of the thin shell, the maximum casting speed to avoid sub-mold bulging cracks in billet casting, and the ideal taper of continuous billet casting molds.

8.1 Summary of CON2D Improvement

The current thermal mechanical is improved based on the previous model [19, 20] to simulate the continuous casting of steel more realistically.

Heat flux at the steel surface is investigated corresponding to different problems as shown in Figure 6.1. The average heat flux profiles are fitted from the measured average heat flux in the mold available in the literature [5–8, 10, 15, 182, 183]. The instantaneous heat flux profiles actually used in the CON2D simulations are obtained by differentiating the corresponding average heat flux function and then applied on the shell surface uniformly around the section perimeter. This approach makes CON2D able to simulate continuous casting processes under realistic heat transfer conditions.

A heat resistor model across the heat flow path from the cooling water to the shell surface is developed for the 2-D simulations to address the interdependence between the heat flux at the shell surface and the gap formed between the shell surface and the mold wall. Note that the gap size also depends on the deformation of the steel. Applying this heat resistor model enables the fully coupled heat transfer and stress analysis of CON2D.

Liquid and solid phase fractions are calculated based on pseudo-binary non-equilibrium Fe-C phase diagram. The phase diagram is abstracted from the fraction temperature curves of a steel predicted by a comprehensive micro-segregation model [2, 167] under given solidification conditions. In order to quantitatively predict hot tear cracks during the continuous casting of steels, previous hot tear criteria are reviewed and evaluated based on their capability and feasibility. An empirical strain criterion [21] is chosen to implement in CON2D to predict hot tear cracks. This empirical criterion bears both essential factors influencing the initiation of hot tear cracks, mushy zone width and the mechanical strain rate, included in the more comprehensive RDG hot tear criterion.

A model representing the mechanical behavior of mushy steel is developed based on a two-phase (liquid and solid) formulation of mass balance and momentum balance equations [138]. Interdendritic flow is modelled by Darcy's law. Three different forms of mushy zone constitutive model are derived for the cases of large permeability $(K \to \infty)$, zero permeability and intermediate permeability $(K \to 0)$, respectively. The mushy zone constitutive equation used follows the large permeability model. This maximizes the inelastic strain in the mushy zone and provides conservative hot tear crack prediction with the empirical hot tear strain criterion.

8.2 Summary of CON2D Applications

8.2.1 Critical Shell Thickness Due to Tensile Rupture

The theoretical limits of the shell thickness, average heat flux and casting speed of the steel continuous casting process as a function of steel grade, section size, and mold length, assuming ideal mold lubrication is investigated. The predictions are based on the minimum heat flow that is just able to produce a thin shell with the critical thickness needed to withstand the ferrostatic pressure below the mold and avoid a longitudinal rupture from excessive inelastic stain.

The critical shell thickness is predicted to be on the order of 3mm. It is surprisingly insensitive to steel grade and superheat, but decreases with decreasing section size and increasing working mold length. The critical average heat fluxes in the mold, which is naturally related to the shell thickness at the mold exit, are predicted to be extremely low, less than $0.4MWm^{-2}$ for a conventional 700mm working mold length, 200mm square bloom mold. This corresponds to a high casting speed of 21m/min with perfect contact between the mold and steel surface or a large 2.2mm oscillation mark depth with a 2.2m/min casting speed for a 700mm length mold.

The infeasibility of these limits in practice is likely due to other problems limiting the casting speed such as sub-mold bulging and local thin shell due to insufficient taper. Attention should return to focussing on these other problems.

8.2.2 Casting Speed Limit Due to Sub-mold Bulging

Higher casting speed leads to a thinner and hotter shell at mold exit and more bulging below the mold. Excessive bulging below mold exit may generate subsurface off-corner longitudinal hot tear cracks due to subsurface tension on the weak solidification front due to hinging around the corner, especially just below mold exit.

Figure 6.19 is a tool for mold designers or operators to determine critical casting speeds for any chosen maximum bulging criterion. For the 0.27%C steel, an empirical fracture criterion for hot tearing based on strain, strain rate and mushy zone temperature range corresponds to 4-10mm maximum bulging. This indicates critical casting speeds of 5m/min for a 120mmsquare section and 800mm mold and 1.5m/min for a 250mm square section and 500mmmold.

As section size increases from 120mm to 250mm, the critical casting speed decreases from 5.0m/min to 1.8m/min for a 800mm mold, due to the higher off-corner subsurface tensile strain caused by larger ferrostatic bending force.

As mold length increases from 600mm to 1100mm, the critical casting speed increases from 3.75m/min to 6m/min for 120mm section size, due to the colder and thicker shell at the mold exit. High tensile stresses build up at the billet corner may contribute to transverse corner cracks due to high corner cooling. With the ideal taper and alignment assumed here, these cracks appear not to limit casting speed.

Billet casting productivity is limited by off-corner subsurface hot tear cracks to around 1 tonne per minute. Increasing section size billet does not produce a significant advantage in productivity. Longer mold length and sub-mold support, such as properly aligned foot rolls, are recommended to achieve higher productivity.

8.2.3 Ideal Taper of Billet Casting

CON2D has been applied to investigate different mold configuration assumptions including corner behavior in order to predict optimal taper profiles. Several conclusions can be drawn:

- The shape of the mold wall around the billet perimeter should be carefully designed to ensure optimal thermal-mechanical behavior of the billet, especially near its corner. Too little taper leads to hot spot at off-corner location, and increases sub-mold bulging. Longitudinal off-corner sub-surface cracks or even breakouts may happen at extreme conditions. Too much taper overcools the corner region. This makes the billet prone to transverse surface cracks or longitudinal sub-surface cracks. The ideal taper design minimizes surface temperature differences around the billet perimeter. Although accurate taper prediction should consider a full 2-D transverse section, a 1D taper prediction by CON2D with a slice domain is surprisingly accurate even for billet casting molds. Considering its great computational savings, this 1-D method is acceptable for online taper prediction in industry or parametric studies in academia.
- The ideal taper is a function of casting speed and mold length. More fundamentally, it depends on the total heat removed in the mold regardless of the casting speed or mold length. The higher is the total heat extracted by the mold, the larger taper is needed. A 1.4%m⁻¹ taper is needed when the total heat removed by the mold is 90MJm⁻².

When the total heat removed by mold is decreased to $10MJm^{-2}$, almost no taper is needed.

- More taper is needed near the meniscus in order to compensate for the faster initial shrinkage. Therefore, parabolic mold taper or multifold linear taper with larger taper near the meniscus is recommended.
- Mold distortion away from shell increases the need for parabolic or multifold linear taper in billet molds. Mold distortion increases with heat flux in the mold from 0.04% at $1.4MWm^{-2}$ to over 0.4% at $5.6MWm^{-2}$.

8.3 Future Work

The majority of this work is to apply CON2D to investigate three important billet issues related to hot tear cracks, the critical shell thickness to avoid breakouts, the maximum casting speed to avoid off-corner sub-surface cracks, and ideal taper prediction. Improvements of CON2D has been made to assist these objectives. Mushy zone constitutive model development has been initiated to make better predictions of mushy zone mechanical behavior and hot tear cracks.

Future work is suggested as follows:

Continue the development of constitutive model of the mushy zone. Development will focus on three aspects: permeability model and the CON2D implementation. The permeability model is essential to predict the interdendritic flow in the mushy zone. Steel permeability experiments and models are very limited. So is the mechanical behavior. Therefore, experimental investigation of mushy steel permeability and mechanical behavior are needed. The permeability study should investigate the effect of several important factors, such as the primary and secondary dendrite arm spacings, liquid fraction and grain size. Implementing the mushy zone model with small permeability (*K*→ 0) enables CON2D to predict realistic stress, strain as well as the interdendritic

liquid pressure in the mushy zone. However, the difference of the behaviors between the solid and the mushy zone makes the stress model more difficult to converge. Therefore, small element size is needed near the solidification front in the mushy zone. As the solidification front moves through the whole modeling domain, local refinement around the mushy zone by adaptive meshing technique is preferred to get both enough mesh refinement in the mushy zone and low computation cost.

- A better hot tear criterion should be developed to predict hot tear cracks more accurately. Upon the completion of the mechanical model of the mushy zone, new hot tear criterion that is more comprehensive than the RDG criterion can be implemented in CON2D based on the mushy zone stress, strain and interdendritic liquid pressure. This new criterion should take more physical phenomena into account, such as grain sizes, dendrite structure (columnar or equixed). Microsegregation model should also extend below solidus to include precipitation effects. Fundamental-based dimensional analysis should be conducted during the criterion development to determine the importance of each physical quantity before incorporating it into the criterion. This will also lead to a unit independent criterion with clearer physical representations.
- Fully coupled heat transfer and stress model should be further developed to include the mold into CON2D. This makes CON2D able to predict the gap between the mold wall and shell surface with better accuracy. Moreover, multi-dimensional mold distortion, mold stiffness, and multi-dimensional mold taper can be considered in CON2D, in order to simulate the continuous casting process more realistically.
- Ideal taper prediction should be extended based on the results of the current work to investigate the 2-D ideal taper. In the current work, a controlled small gap is preferred to generate uniform surface temperature around the strand section perimeter to avoid both in-mold corner surface cracks and sub-mold off-corner sub-surface cracks. However, the current work still assumes a straight mold wall around the section perimeter.

Although this straight mold is also able to be tapered to control the gap around strand corner, the center of the mold will squeeze the steel surface and increase the friction between the mold and steel. This could be avoided by using a curved shape around the section perimeter followed right shrinkage of the strand.

• In addition to the critical shell thickness to avoid breakouts and the maximum casting speed to avoid off-corner inner cracks due to bulging, there are other issues to be investigated such as the axial strain and withdraw force, the effect of the secondary cooling pattern, and sub-mold roll support pattern and alignment.

Appendix A. Finite Element Implementation of the Heat Transfer Model

A.1 Linear Temperature Triangles

The small triangle in Figure A.1 show the constant temperature-gradient triangle element used for the heat flow model. Temperature within an element is interpolated by the same shape functions used to interpolate the coordinates.

$$T = \sum_{i=1}^{3} N_i(x, y) T_i$$
 (A.1)

The [B] matrix in global coordinate system can be obtained as:

$$[B] = \frac{1}{2A} \begin{bmatrix} y_2 - y_3 & y_3 - y_1 & y_1 - y_2 \\ x_3 - x_2 & x_1 - x_3 & x_2 - x_1 \end{bmatrix}$$
(A.2)

where A is the area of the triangle element.

A.2 Conductance Matrix and Capacitance Matrix

The elements in conductance matrix and the capacitance matrix in Equation 4.15 are given in Equations A.3 and A.4. Refer to Cook [190] for the details of the area integration of the natural coordinate function.

$$[K]_{el} = \int [B]^T \begin{bmatrix} k_e & 0 \\ 0 & k_e \end{bmatrix} [B] dA$$
(A.3)
$$[C]_{el} = \frac{\rho c_p A}{12} \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix}$$
(A.4)



Fig. A.1: Six-node quadratic displacement triangle element with Gauss points for stress model with corresponding four three-node linear temperature triangle elements for heat flow model

where k_e is the average conductivity of the three nodal values within each element, and c_p is the effective specific heat within an element given in Equation 4.16.

Appendix B. Finite Element Implementation of the Stress Model

B.1 Linear Strain Elements

Figure A.1 shows the six-node linear strain isoparametric triangle finite element used in this work. Global coordinates and displacements within each element are interpolated from its nodal values by:

$$\begin{cases} x \\ y \end{cases} = \sum_{i=1}^{6} \begin{bmatrix} N_i & 0 \\ 0 & N_i \end{bmatrix} \begin{cases} x_i \\ y_i \end{cases}$$
(B.1)

$$\left\{ \begin{array}{c} u \\ v \end{array} \right\} = \sum_{i=1}^{6} \left[\begin{array}{c} N_i & 0 \\ 0 & N_i \end{array} \right] \left\{ \begin{array}{c} u_i \\ v_i \end{array} \right\}$$
(B.2)

where the shape function in natural local coordinates are:

$$\begin{bmatrix} N_1 & N_2 \dots N_6 \end{bmatrix} = \\ s(2s-1) & t(2t-1) & r(2r-1) & 4st & 4tr & 4sr \end{bmatrix}$$

$$r = 1 - s - t$$
(B.3)

B.2 Generalized Plane Strain Formulation

The three unknowns, a, b, and c, which describe the out-of-plane strain in Equation 4.5, are assembled into the finite element Equations to solve concurrently with the in-plane displacements. The displacement vector used for this condition is therefor:

$$\{\delta_{15\times 1}\} = \left\{ \begin{array}{ccc} \{u_{12\times 1}\}^T & a & b & c \end{array} \right\}^T$$
where
$$\{u_{12\times 1}\} = \left\{ \begin{array}{ccc} u_1 & v_1 & \dots & u_6 & v_6 \end{array} \right\}^T$$
(B.4)

where $u_{12\times 1}$ is the classic displacement vector. The strain-displacement relationship is:

$$\left\{ \begin{array}{ccc} \Delta \epsilon_x & \Delta \epsilon_y & \Delta \epsilon_{xy} & \Delta \epsilon_z \end{array} \right\}^T = \left[B'_{4 \times 15} \right] \{\delta\} \tag{B.5}$$

where $[B_{4\times 15}^{'}]$ matrix for the 2D generalized plane strain configuration is given as:

$$\begin{bmatrix} B'_{4\times 15} \end{bmatrix} = \begin{bmatrix} B_{3\times 12} & [0_{3\times 3}] \\ [0_{1\times 12}] & 1 & x & y \end{bmatrix}$$
where
$$\begin{bmatrix} \frac{\partial N_1}{\partial x} & \cdots & \frac{\partial N_6}{\partial x} & 0 & \cdots & 0 \\ 0 & \cdots & 0 & \frac{\partial N_1}{\partial y} & \cdots & \frac{\partial N_6}{\partial y} \\ \frac{\partial N_1}{\partial y} & \cdots & \frac{\partial N_6}{\partial y} & \frac{\partial N_1}{\partial x} & \cdots & \frac{\partial N_6}{\partial x} \end{bmatrix}$$
(B.6)

The elastic-strain relation is:

$$\begin{bmatrix} \Delta \sigma_x \\ \Delta \sigma_y \\ \Delta \sigma_{xy} \\ \Delta \sigma_z \end{bmatrix} = [D] \left(\begin{cases} \Delta \epsilon_x \\ \Delta \epsilon_y \\ \Delta \epsilon_{xy} \\ \Delta \epsilon_z \end{cases} - \begin{cases} \Delta \epsilon_T \\ \Delta \epsilon_T \\ \Delta 0 \\ \Delta \epsilon_T \end{cases} - \begin{cases} \Delta \epsilon_{plx} \\ \Delta \epsilon_{ply} \\ \Delta \epsilon_{ply} \\ \Delta \epsilon_{plx} \end{cases} \right)$$
(B.7)

The deviatoric stress vector is:

$$\{\sigma\}' = \left\{ \begin{array}{ll} \sigma_x - \frac{1}{3}\sigma_m & \sigma_y - \frac{1}{3}\sigma_m & \sigma_z - \frac{1}{3}\sigma_m & \tau_{xy} \end{array} \right\}$$
where
$$\sigma_m = \sigma_x + \sigma_y + \sigma_z$$
(B.8)

The von-Mises or "equivalent" stress is:

$$\bar{\sigma} = \sqrt{\frac{3}{2} \left((\sigma_x - \sigma_y)^2 + (\sigma_x - \sigma_z)^2 + (\sigma_z - \sigma_y)^2 + 2\tau_{xy}^2 \right)}$$
(B.9)

B.3 Global Stiffness Matrix and Force Vectors

The global stiff matrix [K], and force vectors, $\{\Delta F_{\epsilon_{th}}\}$, $\{\Delta F_{\epsilon_{in}}\}$, $\{F_{fp}\}$, and $\{F_{el}\}$ in Equation 4.21 are assembled from the local stiffness matrix and force vectors of each element at the current time step, t.

$$[K] = \sum_{e=1}^{n} \int_{A_e} \left([B]_e \right)^T [D] [B]_e dA \tag{B.10}$$

$$\{F_{fp}\} = \sum_{e=1}^{n-1} \int_{L_{fp}} \left([N]_e \right)^T (F_p) \, dL_{fp} \tag{B.11}$$

$$\{\Delta F_{th}\} = \sum_{e=1}^{n} \int_{A_e} \left([B]_e \right)^T [D] \{\Delta \epsilon_{th}\} dA$$
(B.12)

$$\{\Delta F_{in}\} = \sum_{e=1}^{n} \int_{A_e} \left([B]_e \right)^T [D] \{\Delta \epsilon_{in}\} dA$$
(B.13)

$$\{\Delta F_{el}\} = \sum_{e=1}^{n} \int_{A_e} \left([B]_e \right)^T [D] \{\Delta \epsilon_{el}\} dA$$
(B.14)

Integrals are evaluated numerically using standard second order Gauss quadrature [190] according to the integration sampling points given in Figure A.1 with constant weighting fractions of 1/3.
Appendix C. Sweeping Algorithm

The algorithm is described as follows and schemed in Figure C.1:

Find out the intersection point, S, between an axis (either x, y, or z) and the plane perpendicular to the given vector, d_3 described in Equation 4.51, that passes an arbitrarily chosen point, P. Take vector from P to S, d_4 , as the base sweeping vector and find out a new vector, d_5 , that is cross orthogonal with respect to d_3 and d_4 .

$$\boldsymbol{d}_5 = \boldsymbol{d}_3 \times \boldsymbol{d}_4 \tag{C.1}$$

Use d_4 and d_5 to find out all equally distributed sweeping vectors.

$$d_{sij} = d_{4j}\cos\theta + d_{5j}\sin\theta$$

$$j = x, y, z$$
(C.2)

 θ is the angle between d_4 and d_{si} .



Fig. C.1: Sweeping algorithm

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Author's Biography

Chunsheng Li was born on January 26, 1971 in Beijing, China. After completing his Bachelor's degree with honors in the Automotive Engineering Department at Tsinghua University, Beijing, China in 1994, he was employed as a Programming Engineer at HITACHI Huasun Information System Co. Ltd. for two years. In the Fall of 1996, he began to pursue his graduate study in the Department of Mechanical Engineering at the University of Illinois at Urbana-Champaign. He completed his Master of Science degree advised by professor Henrique Reis in 1998.

Under the guidance of Professor Brian G. Thomas, he has worked on thermal stress modeling of continuous casting of steels for his Ph.D. program at the Mechanical and Industrial department. His research interests are in the areas of mathematical modeling of thermal and mechanical behaviors of solidification process and hot tear cracks prediction. He extended his knowledge and experience of steel casting and hot tearing crack prediction out of the university by conducting a research project at Champaign Simulation Center, Caterpillar Co. supervised by Caterpillar Technical Service Center and professor Brian G. Thomas.

Chunsheng also has knowledge in many other areas such as control theory, signal processing and computational science. Following the completion of his Ph.D, Chunsheng Li will begin to work for Caterpillar Inc. as a senior development engineer.