Hydrogen Pore Formation in an Al-Si Alloy – an Examination of the Role of Hydrogen Macrosegregation

by

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Abstract

Porosity related defects are one of the leading causes of cast rejection in casting industry since they are detrimental to the fatigue performance of the cast components, primarily when the pores are located in an area of high cyclic stress or located near the surface. Many efforts have been made to develop computational models that predict pore formation. However, one aspect of microporosity formation that has previously not been considered in detail is the effect of macrosegregation of hydrogen. Towards this goal, the user-defined scalars and corresponding user-defined functions were developed to account for hydrogen macrosegregation during solidification of low pressure die casting (LPDC) of A356 aluminum alloy wheels. Numerical simulation of the LPDC process has been implemented within the commercial CFD software package, FLUENT 16.0. The model has been validated against temperature and microstructural data taken from a commercially cast wheel. The amount of species (silicon and hydrogen) segregation in the wheel has been shown to be significant in the rim/spoke junction. The output data from the FLUENT model were then fed into the in-house microporosity model to predict pore size distribution at discrete locations.

The in-house microporosity model has been updated to incorporate the effects of hydrogen macrosegregation, cooling rate and local pressure drop on pore size distribution in the wheel cast. The microporosity model used a Gaussian function of hydrogen supersaturation in the melt to simulate nucleation site distribution and assumed pore growth was controlled by hydrogen diffusion process and besides, the model took into account pore growth associated with liquid encapsulation at a high solid fraction. The samples from a cast wheel have been analyzed using X-rayed microtomography to provide basic validation to the microporosity model. The predicted results showed that the evolution in pressure has the dominant effect on pore growth, but only
under conditions where pores have nucleated prior to the abrupt pressure drop. Otherwise, the cooling rate appears to have the dominant effect. The model prediction shows pore size increases with decreasing pressured drop and cooling rate.
Lay Summary

One of the on-going challenges in the automotive industry is to control defects so as to improve product quality and reduce production cost. Microporosity related defect is one of the main causes of cast rejection in the automotive industry since they are detrimental to the fatigue performance of the wheel, primarily when the pores are located in an area of high cyclic stress. The particular emphasis of the research is to develop a methodology to quantitatively describe hydrogen macrosegregation during solidification of the Low Pressure Die Casting of A356 aluminum alloy wheel and investigate its impact on hydrogen-based microporosity formation. The implications of accounting for the effect of hydrogen macrosegregation on prediction in microporosity formation include an improved ability to predict fatigue performance of the casting.
Preface

My contributions and other works that I used are summarized as follows:

In Chapter 4, I developed the prototyped model of L-shape casting and user-defined functions (subroutines) capable of simulating hydrogen macrosegregation.

In Chapter 5, the geometry of both wheel and the dies used in the LPDC model was provided by Dr. Carl Reilly (Research Associate of the Department of Materials Engineering at University of British Columbia). I assembled and meshed the computational domain. In addition, I referred to the input file of his ABAQUS model to assign the boundary conditions to the LPDC model. The XMT analysis was performed by Professor Andre Phillion (one of my co-supervisors, Associate Professor in Department of Materials Science and Engineering at McMaster University) in the United Kingdom. I conducted XMT data analysis to characterize the porosity size distribution in each sample in ImageJ. The microporosity model was initially developed by Dr. Lu Yao (Research Associate of the Department of Materials Engineering at University of British Columbia) in Fortran. I updated the code in Python so as to include the effect of hydrogen macrosegregation on porosity formation and pore growth associated with liquid encapsulation at a high solid fraction.

This following accepted manuscript is included in Chapters 5:


I was responsible for the drafting this paper, and my co-authors gave a close review of the manuscript and useful suggestions. Section 5.1 and 5.2 included the contents presented in the publication.
# Table of Contents

Abstract .................................................................................................................................................. ii

Lay Summary ........................................................................................................................................ iv

Preface ................................................................................................................................................ v

List of Tables ....................................................................................................................................... ix

List of Figures ....................................................................................................................................... x

List of Symbols ..................................................................................................................................... xvi

List of Abbreviations .......................................................................................................................... xix

Acknowledgements .............................................................................................................................. xx

1 Introduction ......................................................................................................................................... 1

1.1 Wheel Casting Process .................................................................................................................. 3

1.2 Porosity in Aluminum Alloy Wheels ........................................................................................... 4

1.2.1 Macroporosity .......................................................................................................................... 4

1.2.2 Microporosity ........................................................................................................................... 5

2 Literature Review .............................................................................................................................. 8

2.1 Solidification Behavior of A356 .................................................................................................... 8

2.1 Microsegregation ............................................................................................................................ 11

2.1.1 Lever Rule ............................................................................................................................... 13

2.1.2 Scheil Model ............................................................................................................................ 14

2.1.3 Brody and Flemings Model ....................................................................................................... 14
2.2 Macrosegregation .............................................................................................................. 15
  2.2.1 Analytical Solutions .................................................................................................. 16
  2.2.2 Numerical Models .................................................................................................. 17
2.3 Porosity Prediction ........................................................................................................ 20
  2.3.1 Hydrogen-based Pore Nucleation .......................................................................... 20
  2.3.2 Hydrogen-based Pore Growth ................................................................................ 23
  2.3.3 Microporosity Models ............................................................................................. 24
3 Project Objectives and Scope ......................................................................................... 28
4 Model Development ......................................................................................................... 31
  4.1 Description of The Methodology for Numerical Simulation .................................... 32
    4.1.1 Mass Continuity Equation .................................................................................... 33
    4.1.2 Momentum Conservation Equation ...................................................................... 35
    4.1.3 Energy Conservation Equation ............................................................................ 37
    4.1.4 Species Conservation Equation ............................................................................ 38
  4.2 Hydrogen Species Conservation .................................................................................. 40
  4.3 Porosity Model ............................................................................................................. 41
  4.4 Simplified Model of L-Shaped Cross-section Casting of A356 ................................. 43
  4.5 Sensitivity Analysis ..................................................................................................... 60
    4.5.1 The Effect of Cooling Conditions ......................................................................... 60
    4.5.2 The Effect of Velocity Attenuation ....................................................................... 64
4.5.3 The Effect of Body Force ................................................................. 71
4.5.4 The Effect of Mesh Size ................................................................. 74
4.5.5 The Effect of Time Step Size ......................................................... 76
4.6 Updates to the Hydrogen-Based Pore Model ................................... 78
4.7 Microporosity Prediction in L-shaped Casting ................................. 82
4.8 Sensitivity Analysis on the Updated Porosity Model ......................... 84
  4.8.1 The Effect of Hydrogen Concentration in Liquid ($C_{H,liq}$) ........... 84
  4.8.2 The Effect of Velocity Attenuation Parameter ($A_{mush}$) ............. 88
  4.8.3 The Effect of Critical $f_s$ ............................................................. 89
  4.8.4 The Effect of Thermal Boundary Conditions ............................. 91
5 Low Pressure Die Casting Process ..................................................... 98
  5.1 LPDC Model Development ............................................................ 98
  5.2 Result and Discussion .................................................................. 108
6 Summary, Conclusions and Future Work ......................................... 140
References .......................................................................................... 144
Appendix ............................................................................................. 151
List of Tables

Table 2.1 Chemical composition in weight percent of A356[13] ................................................. 8
Table 4.1 Thermo-physical properties used in the numerical model ............................................ 45
Table 4.2 Boundary conditions used in the numerical models ..................................................... 61
Table 5.1 Thermophysical properties used in the numerical model ............................................. 101
Table 5.2 Interfacial heat transfer coefficient at wheel/die interfaces ......................................... 104
Table 5.3 Combined convection/radiation boundary condition .................................................... 105
Table 5.4 Cooling channel boundary conditions ........................................................................ 107
Source code for the UDFs ............................................................................................................. 151
List of Figures

Figure 1.1 Assemblies for LPDC process[8] ................................................................. 3
Figure 1.2 Macroporosity cluster in rim/spoke section[8] .............................................. 4
Figure 1.3 Solubility of Hydrogen at atmospheric pressure in aluminum[10] ..................... 6
Figure 1.4 Evolution of microporosity in directionally solidified aluminum alloy[12] ............ 7
Figure 2.1 Al-Si phase diagram[14] .............................................................................. 9
Figure 2.2 Plot of evolution of solid fraction of unmodified A356 with temperature and its first derivative at 0.52°C/s[17] ................................................................................. 10
Figure 2.3 The grain structure in directionally solidified Al-7wt% Si casting[18](Left) and schematic for a 2D casting[19](Right) ........................................................................... 11
Figure 2.4 Al-H phase diagram[18] .............................................................................. 12
Figure 2.5 Schematic representation of cellular structure[19] ............................................ 13
Figure 2.6 Schematics of macrosegregation in a killed steel ingot. + denotes positive segregation and – denotes negative segregation[28] .......................................................... 16
Figure 2.7 Schematics about gas component diffusion into a pore (a) and concentration profile in an ideal spherical geometry (b)[9] .................................................................................. 23
Figure 3.1 Schematic of the overall modelling methodology used to predict pore size distribution for L-shaped and LDPC casting ................................................................ 30
Figure 4.1 Variation of $A_{mush}$ (kg/m$^3$s) with respect to SDAS ($\mu$m) assuming a constant liquid viscosity of 0.0014kg/m$^3$s .......................................................................................... 36
Figure 4.2 Geometry, mesh and boundary conditions of 2-D axisymmetric model .......... 44
Figure 4.3 Solidification sequence ............................................................................... 48
Figure 4.4 Velocity magnitude at 5.5, 8.5 and 15s ........................................................ 49
Figure 4.5 Gauge pressure at 5.5, 8.5 and 15s ................................................................. 50
Figure 4.6 Liquid mass fraction of silicon calculated by FLUENT at 5.5, 8.5 and 15s .......... 51
Figure 4.7 Evolution in solid fraction with temperature (upper plot) and liquid mass fraction of silicon with solid fraction (lower plot) at three locations ......................................................... 52
Figure 4.8 Liquid mass fraction of Si obtained through the UDS method (Left) and calculated by FLUENT (Right) at 5.5s ........................................................................................................ 54
Figure 4.9 Liquid mass fraction of Si obtained through the UDS method (Left) and calculated by FLUENT (Right) at 8.5s ........................................................................................................ 55
Figure 4.10 Liquid mass fraction of Si obtained through the UDS method (Left) and calculated by FLUENT (Right) at 15s ......................................................................................................... 55
Figure 4.11 Comparison of liquid mass fraction of Si obtained through the UDS method and calculated by FLUENT at point 3 .......................................................................................... 57
Figure 4.12 Mass fraction of silicon in solid obtained through the UDS method (Left) and calculated by FLUENT (Right) at 30s ........................................................................................................ 58
Figure 4.13 Comparison of silicon mass fraction in solid profiles along rim centre ............ 59
Figure 4.14 Comparison of silicon mass fraction in solid profiles along spoke centre ......... 60
Figure 4.15 Solidification sequence among three cases ....................................................... 62
Figure 4.16 Silicon mass fraction predicted by three cases near the end of solidification ...... 63
Figure 4.17 Silicon mass fraction predicted after solidification with different levels of attenuation in the mushy zone: (a) $A_{mush} = 10^5$, (b) $A_{mush} = 10^6$, (c) $A_{mush} = 10^7$ and (d) $A_{mush} = 10^8$ .......... 65
Figure 4.18 Silicon mass fraction with different $A_{mush}$ values along rim centre ............... 66
Figure 4.19 Silicon mass fraction with different $A_{mush}$ values along spoke centre .......... 66
Figure 4.20 Variation of velocity with fraction liquid for different $A_{mush}$ at Point 1 .......... 68
Figure 4.21 Variation of velocity with fraction liquid for different $A_{mush}$ at Point 3 ........................ 68
Figure 4.22 Variation of velocity with fraction liquid for different $A_{mush}$ at Point 2: (a) in full velocity (b) expanded view up to $5\times10^{-3}\,m/s$ ................................................................. 69
Figure 4.23 Variation of pressure with fraction liquid for different $A_{mush}$ at point 2 .................. 70
Figure 4.24 Micrographs of a commercial production of A356 wheel at rim/spoke junction ...... 71
Figure 4.25 Comparison of silicon mass fraction at 20s without gravity (Left) and with gravity (Right) .................................................................................................................. 72
Figure 4.26 Comparison of silicon mass fraction along rim centre ............................................. 72
Figure 4.28 Comparison of pressure variation with fraction liquid at Point 2 ............................ 73
Figure 4.29 Silicon mass fraction predicted by FLUENT model at 20s adopting different mesh sizes: a = 2.5$mm$, b = 1.5$mm$, c = 1$mm$, d = 0.75$mm$ ................................................................. 75
Figure 4.30 Pressure as a function of fraction liquid at Point 2 with different mesh sizes............ 76
Figure 4.31 Silicon mass fraction predicted by the model at 20s with different time step sizes: a = 0.0005$s$, b = 0.002$s$, c = 0.01$s$, d = 0.05$s$ ........................................................................................................ 77
Figure 4.32 Pressure as a function of fraction liquid at point 2 with different time step sizes..... 78
Figure 4.33 Nucleation site distribution as a function of hydrogen supersaturation .............. 84
Figure 4.34 Comparison of variation of $C_{H,liq}$ with liquid fraction $f_s$ at point 2:(a) full range in $f_s$, (b) expanded view up to $f_s = 0.6$ ................................................................. 86
Figure 4.35 Comparison of pore size distribution between different approaches .................... 87
Figure 4.36 Predicted porosity volume fraction by different approaches ................................. 87
Figure 4.37 Comparison of pore size distribution among different $A_{mush}$ .............................. 88
Figure 4.38 Comparison of porosity fraction among different $A_{mush}$ ................................. 89
Figure 4.39 Comparison of pore size distribution among different critical solid fractions ....... 90
Figure 4.40 Porosity volume fraction under different critical $f_s$ .......................................................... 91
Figure 4.41 Hydrogen mass fraction as a function of solid fraction among different cases........ 92
Figure 4.42 Temperature as a function of solid fraction among different cases....................... 93
Figure 4.43 Pressure drop as a function of solid fraction at point 2 among different cases : (a) full range in pressure, (b) expanded view up to -4000 Pa................................................................. 95
Figure 4.44 Local pressure and the vapour pressure of hydrogen pore as a function of solid fraction at point 2, Case 2 ........................................................................................................... 96
Figure 4.45 Comparison of pore size distribution among different cases ................................. 97
Figure 5.1 Die and wheel assembly ................................................................................................. 100
Figure 5.2 Expanded view of the mesh within the red circle in Fig.5.1 ........................................ 100
Figure 5.3 Thermocouple locations on various die components ................................................. 108
Figure 5.4 Thermocouple locations within the wheel................................................................. 109
Figure 5.5 Comparison between experimental data (dash) and simulated (solid) temperatures at top die................................................................................................................................. 110
Figure 5.6 Comparison between experimental data (dash) and simulated (solid) temperatures at top die drum core ......................................................................................................................... 110
Figure 5.7 Comparison between experimental data (dash) and simulated (solid) temperature at bottom die ........................................................................................................................................... 111
Figure 5.8 Comparison between experimental data (dash) and simulated (solid) temperature at side die ........................................................................................................................................... 111
Figure 5.9 Comparison between experimental data (dash) and simulated (solid) temperatures in the wheel at location A,B and C. ........................................................................................................... 112
Figure 5.10 Comparison between experimental data (dash) and simulated (solid) temperatures in the wheel at location D and E ................................................................. 112
Figure 5.11 Silicon mass fraction contour predicted by the model at 72s ........................................ 115
Figure 5.12 Solidification sequence from fully coupled model .................................................. 116
Figure 5.13 Original image (Left) and corresponding binary image (Right) ......................... 118
Figure 5.14 Microstructure along the centre line in the wheel (left) and Location on wheel where comparison was made (Right) .................................................................................................................. 120
Figure 5.15 Comparison between experimental data (dots) and simulated (lines) silicon mass fraction in the wheel .......................................................................................................................... 120
Figure 5.16 Microstructure in the rim (left) and location on wheel where comparison were made (Right) ........................................................................................................................................ 121
Figure 5.17 Solidification sequence from thermal only simulation (top) and fully coupled model (bottom) .................................................................................................................................................. 123
Figure 5.18 Sample locations (a) and hydrogen mass fraction contour (b) predicted by the model at 72s .................................................................................................................................................. 125
Figure 5.19 The XMT analysis process .......................................................................................... 127
Figure 5.20 Effect of ‘Dilate’ and ‘Erode’ filter combination on image processing ................ 128
Figure 5.21 3-D characterization of porosity at selected locations ............................................ 130
Figure 5.22 Pore nucleation site distribution .............................................................................. 131
Figure 5.23 3-D characterization of porosity (Left) and comparison between measured and predicted pore size distribution at location 4B, 9T, 9B and 5BT (Right) ......................... 134
Figure 5.24 Hydrogen concentration in liquid as a function of solid fraction at location 4B, 9T, 9B and 5BT; (a) full range in $f_s$, (b) expanded view up to $f_s = 0.6$ ......................................................... 137
Figure 5.25 Pressure drop as a function of solid fraction at location 4B,9T, 9B and 5BT........ 138

Figure 5.26 Comparison between measured and predicted pore size distribution at location 4B
adopting different critical solid fraction ......................................................... 139
List of Symbols

\(k_i\) partition coefficient of species \(i\)

\(C_{H,\text{liq}} \text{(mol/m}^3\text{)}\) hydrogen concentration in the liquid

\(f_s\) solid fraction

\(f_l\) liquid fraction

\(f_p\) pore volume fraction

\(C_{i,0} \text{(mol/m}^3\text{)}\) initial concentration of species \(i\)

\(Fo_s\) Fourier number

\(\vec{v} \text{ (m/s)}\) velocity

\(G \text{ (K/m)}\) thermal gradient

\(\mu_i \text{(Pa} \cdot \text{s)}\) liquid viscosity

\(dp \text{ (N/m}^2\text{)}\) pressure change

\(K \text{ (m}^2\text{)}\) permeability

\(\gamma \text{ (N/m)}\) surface tension

\(\lambda_s \text{ (\mu m)}\) secondary dendrite arm spacing

\(P_{H_2} \text{ (Pa)}\) partial pressure of hydrogen in the liquid

\(\rho \text{ (kg/m}^3\text{)}\) density

\(\rho_l \text{ (kg/m}^3\text{)}\) density of liquid A356

\(\rho_s \text{ (kg/m}^3\text{)}\) density of solid A356

\(A_{\text{mush}} \text{(kg/m}^3\text{.s)}\) velocity attenuation parameter

\(g \text{ (m}^2\text{/s)}\) gravitational acceleration

\(H \text{ (J/kg)}\) enthalpy of the material
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L$ (J/kg)</td>
<td>latent heat</td>
</tr>
<tr>
<td>$T(K)$</td>
<td>temperature</td>
</tr>
<tr>
<td>$T_{\text{liquidus}}(K)$</td>
<td>liquidus temperature</td>
</tr>
<tr>
<td>$T_{\text{solidus}}(K)$</td>
<td>solidus temperature</td>
</tr>
<tr>
<td>$T_{\text{melt}}(K)$</td>
<td>melting temperature of Al</td>
</tr>
<tr>
<td>$N_{\text{nuc}}(mm^{-3})$</td>
<td>number density of the nucleated pores</td>
</tr>
<tr>
<td>$ss (mol/m^3)$</td>
<td>supersaturation of hydrogen in the liquid</td>
</tr>
<tr>
<td>$A (mm^{-3})$</td>
<td>total available nuclei</td>
</tr>
<tr>
<td>$\sigma (mol/m^3)$</td>
<td>variation in potency of nucleation sites</td>
</tr>
<tr>
<td>$ss_0 (mol/m^3)$</td>
<td>average supersaturation for pore nucleation</td>
</tr>
<tr>
<td>$C_{i}^e (mol/m^3)$</td>
<td>equilibrium hydrogen concentration in the liquid</td>
</tr>
<tr>
<td>$K_L (mol/m^3/atm^{1/2})$</td>
<td>equilibrium constant</td>
</tr>
<tr>
<td>$P_a (Pa)$</td>
<td>atmospheric pressure</td>
</tr>
<tr>
<td>$P_h (Pa)$</td>
<td>metallostatic pressure</td>
</tr>
<tr>
<td>$\Delta P_d (Pa)$</td>
<td>pressure drop associated with Darcy source term</td>
</tr>
<tr>
<td>$C_{lp} (mol/m^3)$</td>
<td>hydrogen concentration at the liquid and pore interface</td>
</tr>
<tr>
<td>$l_{\text{diff}} (m)$</td>
<td>thickness of the diffusion boundary layer</td>
</tr>
<tr>
<td>$D_{H,\text{aq}} (m^2/s)$</td>
<td>hydrogen diffusion coefficient in the liquid phase</td>
</tr>
<tr>
<td>$r_p (m)$</td>
<td>pore radius</td>
</tr>
<tr>
<td>$\varphi$</td>
<td>impingement factor</td>
</tr>
<tr>
<td>$R_g (J/mol/K)$</td>
<td>gas constant</td>
</tr>
<tr>
<td>$k (W/m K)$</td>
<td>thermal conductivity</td>
</tr>
</tbody>
</table>
\( m_{Si} \) (K/wt.%)\hspace{1cm} \text{Slope of the liquidus for Al-Si}

\( m_{Mg} \) (K/wt.%)\hspace{1cm} \text{Slope of the liquidus for Al-Mg}

\( \lambda \)\hspace{1cm} \text{relaxation factor or thermal conductivity}

\( a_p \)\hspace{1cm} \text{cell matrix coefficient}

\( V_{vol} \) (m\(^3\))\hspace{1cm} \text{cell volume}

\( m \)\hspace{1cm} \text{impingement factor}

\( \Delta t \) (s)\hspace{1cm} \text{time step size}

\( HTC \) (W/m\(^2\)K)\hspace{1cm} \text{heat transfer coefficient}

\( D_{Si,liq} \) (m\(^2\)/s)\hspace{1cm} \text{Si diffusion coefficient in liquid}

\( D_{Mg,liq} \) (m\(^2\)/s)\hspace{1cm} \text{Mg diffusion coefficient in liquid}

\( D_{Si,sol} \) (m\(^2\)/s)\hspace{1cm} \text{Si diffusion coefficient in solid}

\( D_{Mg,sol} \) (m\(^2\)/s)\hspace{1cm} \text{Mg diffusion coefficient in solid}

\( C_p \) (J/kg/K)\hspace{1cm} \text{specific heat}

\( C_{Si,a} \) (wt.%)\hspace{1cm} \text{mass fraction of silicon in the primary phase}

\( C_{Si,eut} \) (wt.%)\hspace{1cm} \text{eutectic mass fraction of silicon}

\( f_E \)\hspace{1cm} \text{volume or area fraction of the Al-Si eutectic}
<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Definition</th>
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<tbody>
<tr>
<td>CAFE</td>
<td>Corporate Average Fuel Economy</td>
</tr>
<tr>
<td>OECD</td>
<td>Organization for Economic Co-operation and Development</td>
</tr>
<tr>
<td>SDAS</td>
<td>Secondary Dendrite Arm Spacing</td>
</tr>
<tr>
<td>HTC</td>
<td>Heat Transfer Coefficient</td>
</tr>
<tr>
<td>IHTC</td>
<td>Interfacial Heat Transfer Coefficient</td>
</tr>
<tr>
<td>LPDC</td>
<td>Low Pressure Die Casting</td>
</tr>
<tr>
<td>UDS</td>
<td>User Defined Scalar or User Defined Subroutine</td>
</tr>
<tr>
<td>UDF</td>
<td>User Defined Function</td>
</tr>
<tr>
<td>TC</td>
<td>Thermocouple</td>
</tr>
<tr>
<td>XMT</td>
<td>X-ray Microtomography</td>
</tr>
</tbody>
</table>
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Although I am the author, this Ph.D. work is the product of the shared wisdom of my supervisors, colleagues, friends and family members.

I would like to thank Professor Steven Cockcroft for his support and guiding me through the entire Ph.D. study. I am also grateful to my co-supervisor Professor Andre Phillion for his insightful contributions to the discussion on my Ph.D. work. In addition, a special thank you to Professor Daan Maijer for his valuable advice.

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Finally, I want to thank my parents for their unconditional love and support.
1 Introduction

Transportation has a significant effect on many aspects of human society ranging from personal mobility and travel to access to goods and services. The automobile has been the dominant mode of personal transportation since the mid-1900’s in both North America and Europe. Its dominance in transportation in a given country generally scales with the disposable income of the population. In the US, there were roughly 0.8 people for every car, whereas, in China, there are roughly 12 people per vehicle[1]. China, however, accounts for the most substantial increase in automobile use amongst its population[2]. The OECD International Transportation Forum estimates that the number of cars worldwide will reach 2.5 billion by 2050 (up from approximately 1 billion in 2010)[3]. In addition to its widespread adoption, the automobile industry has become one of the most important economic drivers around the world, further underpinning the continued global importance of the automobiles[4].

The widespread and growing use of the automobile is such that it now represents a significant contributor to greenhouse gas emissions (estimates place it in the range of 25-30%) and the associated potential for adverse climate change. Thus, government policymakers are moving to legislate improved vehicle efficiencies. In North America, this is being implemented through requirements for automobile manufacturers to meet Corporate Average Fuel Economy (CAFE) requirements. By 2016 passenger cars must improve to 41 mpg and by 2025 this number is close to 60 mpg[5]. While in Europe Union, the 2015 target was 5.6 liters per 100 km and the new cars in 2021 have to achieve a fuel efficiency of around 4.1 liters per 100 km[6].

According to reference[7], weight reduction is one way to enhance fuel efficiency and it will be an essential component of a comprehensive strategy to meet CAFE targets. Aluminum
alloys are a potential alternative to the use of heavier steel in the automotive industry as some alloy variants offer a higher strength-to-weight ratio than steel, excellent corrosion resistance and are close to steel in terms of cost. Good examples of the current use of aluminum alloy in automobiles include cast engine blocks, cylinder heads, transmission casings and wheels, where it has become the dominant material of choice in these applications. In contrast, there has been comparably little adoption in exposed body panels and structural components of the frame and suspension other than in high-end performance cars. Hence, these areas represent significant opportunities for expanding the use of aluminum alloys across a broader section of the automotive market.

Despite broad market penetration of aluminum alloy in automotive powertrain components and in wheels, manufacturers are under pressure to improve the fatigue performance of these components to allow for operation under higher dynamic loading/stress conditions. In the case of wheels, they represent part of the un-sprung weight, and therefore weight reductions in the wheel derived through operation at higher dynamic stresses will lead to further weight reductions in the suspension system. Most new cars in North America use cast aluminum alloy wheels[8]. As a critical safety component, automotive wheels are required to meet demanding mechanical requirements include impact and fatigue performance targets. Additional properties of importance include air-tightness in the rim section, high-quality surface finish and good geometric and rotational balance, making them one of the more challenging automotive castings to produce[8].

Aluminum alloy castings, in general, are particularly sensitive to the formation of porosity, due to the significant difference in solubility of hydrogen between the liquid and solid and large volumetric shrinkage associated with solidification. This porosity can, in turn, undermine the mechanical performance of the component depending on its size if present in an area that
experiences high dynamic or impact stresses[9]. As a result, considerable effort has gone into understanding and predicting the formation of porosity in aluminum castings.

The focus of this work will be on further understanding the development of porosity in cast aluminum components using automotive wheels as an area of application. Thus, some additional background on aluminum alloy wheel casting is appropriate.

1.1 Wheel Casting Process

The low-pressure die casting (LPDC) process has become the predominant technology for the production of aluminum alloy wheels. A typical LPDC setup is shown schematically in Figure 1.1 and includes the holding furnace, transfer tube, sprue and die assembly.

![Figure 1.1 Assemblies for LPDC process][8]

The LPDC process for the production of wheels is cyclic and begins with the pressurization of the furnace to force liquid metal up into the die cavity through the transfer tube. The liquid metal is then cooled and solidified via heat transfer to the die where the heat is removed through cooling channels located within the die and also to the ambient environment. After solidification is complete, the side dies open and the top die is raised vertically. Due to thermal contraction, the
wheel shrinks on to the top die. The top die is raised and then the wheel is ejected onto a transfer tray rolled beneath the top die. The die is then closed and the cycle restarted. Typical cycle time is 3-5 minutes, depending on whether forced water or air is used as the cooling medium. After casting, the wheels are typically roughly machined, heat treated, finish machined and painted.

1.2 Porosity in Aluminum Alloy Wheels

Porosity can act as stress concentrator and crack growth site thereby degrading the fatigue performance of the component. There are two main types of porosity in wheels: macroporosity and microporosity; the former often also referred to as shrinkage-based porosity and the latter as hydrogen-based porosity.

1.2.1 Macroporosity

Macroporosity occurs in regions in a casting associated with liquid encapsulation due to a lack of sufficient liquid feeding to compensate for the volume change from liquid to solid upon solidification. In the case of wheels, macroporosity is commonly seen at the junction between the rim and spoke, as shown in Figure 1.2.

![Figure 1.2 Macroporosity cluster in rim/spoke section][8]
In wheels, the optimum path for solidification to avoid macroporosity is from the top of the rim (inboard rim flange), down the rim and across the spoke ending at the top of the sprue just prior to the end of the cycle and die opening – so-called “good directional solidification”. Failure to design the cooling system in the die, either by improper placement/size of the cooling channels and/or by improperly controlling the on and off timing of the cooling can result in a loss in directional solidification and the formation of a region of liquid/semi-solid material that becomes encapsulated. This region becomes cut off from a source of liquid metal to feed the volumetric shrinkage associated with solidification (in the range of 6 to 7% for aluminum alloys[10]). As the encapsulated liquid cools and solidifies, the significant pressure drop drives pore growth. Upon cooling, these bubble(s) become the pores observed in the cast product. The size can range from 0.5\( \text{mm} \) to several 10’s of \( \text{mm} \). The size and distribution of these pores depend on the volume and solid fraction of the material that is encapsulated. Liquid encapsulation in a casting can be accurately predicted using computer-based heat transfer simulation models providing the models are capable of accurately describing the heat transfer occurring during casting. The accurate prediction of the size range and distribution of the macroporosity remains a challenge.

### 1.2.2 Microporosity

In contrast to macroporosity, microporosity relates to pores relatively small in scale (usually less than 300\( \mu \text{m} \)[8]). Microporosity occurs either due to inadequate compensatory flow in the mushy zone (semi-solid material) at high fractions of solid and/or the formation of hydrogen bubbles. In the case of the hydrogen-related mechanism, it is well known that the solubility of hydrogen in liquid aluminum is much higher than in the solid. Figure 1.3 shows the variation in hydrogen solubility with temperature for pure aluminum and illustrates the large drop in solubility associated with transitioning from the liquid phase to the solid. In addition, due to its high chemical affinity for oxygen, aluminum is capable of decomposing water vapour in the atmosphere and
absorbing the hydrogen. Thus, aluminum is prone to picking up hydrogen when held in the liquid state particularly under warm and humid conditions.

![Graph showing solubility of hydrogen in aluminum](image)

**Figure 1.3 Solubility of Hydrogen at atmospheric pressure in aluminum[10]**

Upon solidification, hydrogen will be rejected from solid into surrounding liquid. When the hydrogen concentration, or more specifically, the activity of hydrogen in the liquid exceeds its local solubility plus an additional amount to overcome nucleation, a hydrogen bubble will form. Figure 1.4 shows an X-ray radiograph of hydrogen pores forming in the inter-dendritic liquid in a directionally solidified sample of an aluminum alloy. In the past few years, a number of good models have been presented in the literature[11] and then validated, to describe methods for predicting hydrogen pore formation in aluminum alloys.
Despite a significant amount of work in understanding and predicting porosity formation in Al-shape casting, there are areas that would benefit from additional work. One such area is the role of macro-segregation of hydrogen. This project will focus on developing a numerical model capable of predicting the role of hydrogen redistribution (macrosegregation) on hydrogen-based pore nucleation and growth. The model will be validated using data collected from a low-pressure die cast A356 alloy wheel. Areas of specific importance to the proposed research program include solidification behavior of A356, microsegregation phenomena and modelling, macrosegregation phenomena and modelling, and hydrogen pore nucleation and growth phenomena and modelling.
2 Literature Review

This chapter will first briefly discuss the solidification behavior of A356, which is the material used in this project. A review will then be conducted on solute segregation that develops in castings at both the micro and macro-scale. Finally, porosity models that predict hydrogen-based pore nucleation and growth will be reviewed.

2.1 Solidification Behavior of A356

Solidification is a phase transformation process in which liquid turns into a solid phase. For a pure metal, solidification occurs when the temperature reaches the melting point (on cooling) at equilibrium, which is a unique temperature. For alloys, solidification occurs within a temperature range and can involve the formation of one or more solid phases. The material used in this project is cast aluminum alloy A356. The standard chemical composition of A356 alloy in weight percent is indicated in Table 2.1. Since Si is the dominant alloy addition, looking at the Al-Si phase diagram (Figure 2.1) provides some insight into the solidification behavior of A356. It can be seen that the composition of Si in A356 is lower than the eutectic composition (12.6wt.%) and higher than the maximum solid solubility of Si in α phase (1.65wt.%). Therefore, A356 is a hypoeutectic alloy and the solidified structure will be comprised of approximately 50% volume fraction primary α-aluminum with the balance comprised of Al-Si eutectic and small amounts of other intermetallics.

<table>
<thead>
<tr>
<th>Composition</th>
<th>Si</th>
<th>Mg</th>
<th>Fe</th>
<th>Ti</th>
<th>Cu</th>
<th>Al</th>
</tr>
</thead>
<tbody>
<tr>
<td>A356</td>
<td>6.5-7.5</td>
<td>0.2-0.45</td>
<td>&lt;0.1</td>
<td>0.12-0.13</td>
<td>&lt;0.002</td>
<td>Bal.</td>
</tr>
</tbody>
</table>
The solidification process in A356 was recently investigated by Thompson[15], who investigated the solidification behavior of both strontium modified and unmodified A356 at different cooling rates. Figure 2.2 shows an example of the measured evolution of solid fraction with temperature for unmodified A356 at a cooling rate of 0.52 °C/s. The peaks in the plot of the first derivative of fraction solid with respect to temperature, arising from the release of latent heat, indicate the formation of the major solid phases. The three phase transformations[16] that were identified are: the formation of α-Al, the formation of primary eutectic Al-Si, and the precipitation of intermetallics Mg2Si.

Figure 2.1 Al-Si phase diagram[14]
At a cooling rate of 0.52°C/s, primary α-Al starts to solidify at around 614°C. The development of binary eutectic occurs at around 575°C. At around 554°C, precipitation of Mg2Si begins and the solidus temperature is reached at around 537°C. Depending on the cooling rate and whether a modifier is added to the alloy, the solidification temperature range changes. Increasing the cooling rate depresses the liquidus temperature, primary eutectic start temperature and the solidus temperature. Addition of alloying elements for grain refinement and modification were found to also have the same effect[15].

In the absence of a grain refiner, the solidified microstructure that develops in A356 is typical of that shown schematically on the right-hand-side of Figure 2.3. In order of formation, the structure consists of an equiaxed (chilled) structure adjacent to the surface of primary heat extraction, a columnar structure and finally an equiaxed structure. A corresponding example of a directionally solidified Al-7wt.%Si alloy is shown on the left-hand-side of Figure 2.3.
Generally, A356 is cast with the addition of a grain refiner such as TiB₂[20], which results in the formation of fine equiaxed structure throughout the casting. In addition, in order to improve mechanical properties of the casting, an alloy (eutectic) modifier such as sodium (Na) or strontium (Sr) is typically also added to the melt to change eutectic morphologies from acicular to fibrous. In the last decade, Sr has become the dominant modifier owing to the fact that it is less chemically reactive than Na, which usually experiences rapid loss from the melt due to volatilization and oxidation[21].

2.1 Microsegregation

Microsegregation refers to compositional inhomogeneities occurring at the scale of the microstructure. It is driven by differences in solute solubility between the solid that is forming and the liquid. Solute is rejected from the solid to liquid (normal segregation) if the equilibrium segregation coefficient \( k_i \) is less than one, where \( k_i \) is defined as follows:
\[ k_i = \frac{C_{i,\text{sol}}}{C_{i,\text{liq}}} \]

Equation 2.1

where the subscript \( i \) refers to the solute species segregating. For example, for Si in Al, \( k_{\text{Si}} = 0.13 \).

In some cases, segregation is said to occur inversely and \( k_i \) is greater than one, i.e. the solubility of solute \( i \) is higher in the solid than that in the liquid. It should be noted that segregation can also occur with respect to dissolved gases in solution. For example, as shown in the Al-H phase diagram (see Figure 2.4), for H in Al, \( k_{\text{H}} = 0.056 \).[22]

In the study of segregation, various analytical models have been developed based on conservation of mass. In the context of their application to microsegregation, the mass balance is based on a volume element representative of the microstructure being studied. For example, directional solidification is occurring in a volume element, perpendicular to two cells, as shown in Figure 2.5. These analytical models assumed various scenarios with respect to the rates of diffusion.
within the solid and the liquid phases and no advective transport of solute in or out of the grain envelope.

![Figure 2.5 Schematic representation of cellular structure][19]

### 2.1.1 Lever Rule

The Lever rule, or equation, is the simplest microsegregation model and assumes infinite solute diffusion in both liquid and solid, i.e. $D_{\text{sol}} = D_{\text{liq}} = \infty$, where $D_{\text{sol}}$ and $D_{\text{liq}}$ ($m^2/s$) are the solute diffusivities in solid and liquid phases, respectively. Thus, the solute is uniformly distributed in each phase at a given solid fraction or temperature. The solute composition (unit: weight percent) in the solid can be expressed as:

$$C_{i,\text{sol}} = \frac{k_i C_{i,0}}{1 - (1 - k_i) f_S}$$

Equation 2.2[23]

where $C_{i,0}$ is the initial solute composition in weight percent, $k_i$ is equilibrium segregation coefficient and $f_S$ is solid fraction. This equation is valid for $C_{\text{sol},i} \leq C_{\text{sol},M}$ (maximum solid solubility in $\alpha$ phase). The Lever rule is consistent with equilibrium solidification conditions, i.e. the conditions in which solidification is proceeding very slowly. Thus, there is adequate time for complete diffusion in the liquid and solid to occur. *Note: the result is a uniform, but not equal,*

---

[19]: #
distribution of solute in the solid and liquid at a given temperature in the solidification temperature range.

2.1.2 Scheil Model

The Scheil model is another analytical approach to describe solute microsegregation during solidification. It assumes no diffusion in the solid and infinite diffusion in liquid, i.e., $D_{sol} = 0$, $D_{liq} = \infty$. For most aluminum alloys, the diffusion rate of the solute components in the solid phase is smaller than that in the liquid. For example, the diffusivity of Si in liquid Al ($D_{Si,liq}$) is $4.75 \times 10^{-9} \text{m}^{2}/\text{s}$ while diffusivity of Si in solid ($D_{Si,sol}$) is $7.61 \times 10^{-13} \text{m}^{2}/\text{s}$ [24] (for H in Al, $D_{H,liq} = 3 \times 10^{-7} \text{m}^{2}/\text{s}$ at 612°C and $D_{H,sol} = 1.07 \times 10^{-8} \text{m}^{2}/\text{s}$ at 500°C [25]). Therefore, as compared to the Lever rule, the Scheil equation will provide a better description of microsegregation occurring with respect to most of the solute constituents present in Al alloy castings. The resulting variation in solute composition in the solid as a function of solid fraction given by the Scheil Equation is:

$$C_{i,sol} = k_i C_{i,0} \left(1 - f_s\right)^{k_i - 1}$$

Equation 2.3[23]

This equation is also valid for $C_{sol,i} \leq C_{sol,M}$. Note: the result is a non-uniform distribution of solute in the solid and a uniform distribution in the liquid at a given temperature in the solidification temperature range.

2.1.3 Brody and Flemings Model

In reality, there is some diffusion occurring in the solid phase. An example of this has been reported in a study on the solidification of Al-4.5wt.%Cu alloy at the cooling rate of 10K/min, in which the author pointed out that diffusion in the solid is not negligible and must be accounted for[9]. An expression for the case where $D_{sol} > 0$ and $D_{liq} = \infty$ was developed by Brody and Flemings[26], which is presented below,

$$C_{i,sol} = k_i C_o \left[1 - \left(2F_{O,k_i}\right) f_s \right]^{\left(k_i - 1\right)}$$

Equation 2.4[23]
where $F_{os}$ is Fourier number for solute diffusion in the solid, and is defined as the ratio of local solidification time to the characteristic time for the diffusion of solute, or:

$$F_{os} = \frac{4D_{sol} \tau_f}{\lambda^2_2}$$

Equation 2.5[9]

In Equation 2.5, $\tau_f$ is local solidification time (s), $D_{sol}$ is solute diffusion coefficient ($m^2/s$) in the solid, and $\lambda_2$ is secondary dendrite arm spacing ($\mu m$). This Fourier number is also referred to as the back diffusion coefficient. *Note:* Equation 2.4 reduces to Scheil equation when $F_{os} = 0$ and to Lever equation when $F_{os} = 0.5$.

### 2.2 Macrosegregation

Macrosegregation occurs as a result of redistribution of solute outside of the grain envelope. The two mechanisms that contribute to the macrosegregation are: bulk liquid motion and bulk solid motion[9][27]. Liquid movement, for example, can arise from forced convection, due to pouring, mechanical stirring or from buoyancy forces induced due to thermal and/or solutal gradients. In addition, the liquid movement can be induced by solidification shrinkage as a result of variation in density between the solid and liquid phases. Solid movement, on the other hand, can be caused by deformation of the mushy zone or grains moving with different velocity than the liquid, i.e. equiaxed gains sedimentation or floating. Solubility differences between the solid and liquid phases, resulting in depletion or enrichment of the liquid or solid, in combination with bulk motion of either phase may result in differences in concentration of the alloy constituent at the scale of the cast component. One important difference between microsegregation and macrosegregation is that macrosegregation cannot generally be removed by a homogenization heat treatment and consequently, can result in significant variation in the physical and mechanical
properties within the cast component. In addition, these inhomogeneities can often be carried over into wrought product. Figure 2.6[28] shows various types of macrosegregation encountered in large, static cast steel ingots. The positive macrosegregation (increase in solute concentration) at the top, or the A-type, comes from buoyancy-driven fluid flow (the advection of lighter solute-rich liquid). The negative segregation (zones deplete in solute) at the bottom is the result of heavier equiaxed crystals, deplete in solute, settling to the bottom of the ingot.

![Figure 2.6 Schematics of macrosegregation in a killed steel ingot.](Image)

Of the different drivers for the fluid flow leading to macrosegregation, solidification shrinkage, thermal buoyancy, and solutal buoyancy are relevant to this study. An analytical solution for macrosegregation driven by liquid flow due to shrinkage is reviewed first, followed by numerical models that simulate macrosegregation driven by shrinkage and/or buoyancy.

### 2.2.1 Analytical Solutions

Flemings et al.[29] investigated solute redistribution due to 1-D interdendritic flow through a volume element containing a fixed dendrite network. Their solution is presented in Equation 2.6. The assumptions include: (i) there is no solute diffusion in the solid; (ii) the density in the liquid and solid are constant, but not equal; (iii) diffusion in the liquid in the direction of fluid flow is
insignificant in comparison to advective transport and can be neglected; (iv) local equilibrium prevails at the L/S interface; and (v) microsegregation occurring normal to the direction of fluid flow can be described based on the Scheil equation. The resulting expression is given below,

\[
\frac{df_i}{dC_{i,\text{liq}}} = \frac{(1-\beta)}{(1-k_i)} \left[ 1 + \frac{\nu_i * G}{\partial T/\partial t} \right] f_i \Rightarrow \frac{df_i}{f_i} = \frac{(1-\beta)}{(1-k_i)} \left[ \frac{1 - \frac{\nu_i}{R}}{C_{i,\text{liq}}} \right] dC_{i,\text{liq}}
\]

Equation 2.6

where \( f_i \) is the liquid fraction; \( C_{i,\text{liq}} \) is the liquid solute composition in weight percentage; \( \beta \) is the solidification shrinkage (as a volume fraction); \( k_i \) is the partition coefficient; \( \nu_i \) is the liquid velocity; \( G \) is the thermal gradient; \( \partial T/\partial t \) is local cooling rate; and \( R \) is the liquidus isotherm velocity = - \( (\partial T/\partial t)/G \). The volume element can be treated as a porous media, therefore, Darcy’s law can be employed to calculate interdendritic fluid velocity as a function of pressure gradient,

\[
\bar{v_i} = - \frac{K}{\mu_l} \left( \frac{dP}{dx} - \rho_l \bar{g}_s \right)
\]

Equation 2.7

where \( \mu_l \) is liquid viscosity; \( \frac{dP}{dx} \) is pressure gradient in x-direction; \( \rho_l \) is density of the liquid; \( \bar{g}_s \) is the gravity vector ; \( K \) is permeability, which is strongly dependant on the volume fraction of solid, and is given by Carman-Kozeny relation[9]:

\[
K = \frac{\lambda_z^2}{180} \frac{(1-f_s)^3}{f_s^2}
\]

Equation 2.8

where \( f_s \) is the volume fraction of solid and \( \lambda_z \) is secondary dendrite arm spacing. The analytical solution for \( C_{i,\text{liq}} \) can be obtained by the integration of Equation 2.6.

2.2.2 Numerical Models

The shortcomings of the above analytical solution include the fact that it is restricted to 1-D and steady-state solidification conditions, and that advective flow in the liquid metal ahead of the liquidus isotherm at the boundary of mushy zone is not included. In the early 1980s, Ridder et
al. [30] proposed a two-phase model that coupled fluid flow in the bulk liquid and interdendritic flow in the mushy zone. The predicted solute redistribution pattern under axisymmetric conditions was in good agreement with experiment results. However, tracking the solid and liquid interface proved to be problematic. In the late 1980s, continuum models based on mixing theory or volume averaging were developed by a number of researchers including Incropera et al. [31], Voller et al. [32] and Beckermann et al. [33]. In these models, one set of transport equations was used to solve the momentum, heat and mass conservation equations in the domain, which at any time consisted of one or more liquid and solid phases. Modeling of macrosegregation was significantly improved by this phase averaging approach. Initially, these macrosegregation models were mainly applied to Al-Cu alloys. For instance, Rousset et al. [34] developed a finite-difference based numerical model to predict inverse segregation during the directional solidification of an Al-Cu alloy. The results showed that inverse segregation was related to liquid feeding in the mushy zone, which compensated for solidification shrinkage. This model was extended by Stefanescu et al. [35], such that the solidification process was divided into two stages. In stage 1, the formation of equiaxed grains was modeled whereby the grains then move along with the liquid, therefore, \( \vec{v} = \vec{v}_l \), where \( \vec{v} \) represents velocity. In stage 2, the dendrite skeleton prevents solid movement (i.e. \( \vec{v}_s = 0 \)) and the liquid was modeled as flowing through a stationary dendrite mushy zone. This approach allowed for consideration of the species flux due to relative phase movement. The results demonstrated that solidification shrinkage has a stronger effect on fluid motion in the mushy zone as compared to buoyancy. In another study, Ahmad et al. [36] applied in-house codes based on both the finite volume and the finite element methods to solve conservation equations for mass, momentum, heat and solute. In this work, macrosegregation of two Pb-Sn alloys during solidification was predicted in a rectangular cavity. Fluid flow in these models was driven solely
by thermo-solutal convection. Although there were slight differences in the predicted solute segregation patterns between the finite volume and finite element methods, the results from both simulations were in fairly good agreement with experimental results obtained by Hebditch and Hunt[37].

The models described above have provided for new insights into macrosegregation. However, they have only been applied to simple geometries, contained additional simplifying assumptions, and partially lacked experimental validation. Beckermann et al.[38] extended application of the model described in [33] from binary alloys to multi-component alloys in order to examine the effect of solutal-thermal convection on multi-component alloy macrosegregation. The model was developed on the basis of a volume averaged two-component model, and included diffusion in the solid. The results showed that a good approximation for the macrosegregation pattern could be achieved even when only solving the governing equations for a subset of elements, as long as the chosen elements give rise to significant fluid driving force as a result of their segregation. A fully coupled model[39], consisting of macroscopic mass, heat and momentum balance, microsegregation model and phase diagram calculation module, was developed to simulate the macrosegregation of multi-component aluminum alloys (Al-Cu-Mg) during direct chill casting. A 2-D axisymmetric domain was used and both shrinkage and buoyancy driven flow as well as microsegregation described by either the Lever rule or Scheil equation was developed. The simulated results were found to be in reasonable agreement with experimental data although the effect of solid grain advection was neglected. Recently Ellingsen et al.[40] developed in-house ALSTRUC model, a multi-component microsegregation model, which accounts for multicomponent phase diagram, solid diffusion and growth of secondary phases which are precipitated from the liquid phase. Accurate macrosegregation prediction can be achieved by
coupling the ALSTRUC model with macroscopic transport model. The coupled model was tested on an industrial direct chill casting billet of 6xxx alloy to investigate the effects of solidification shrinkage, thermal and solutal convection and surface exudation on species macrosegregation. The model prediction of species macrosegregation matched the measurement along the centre to the surface of the billet.

The numerical model is becoming a reliable tool to predict the temperature and flow fields in casting processes providing sufficient effort is invested in boundary condition formulation and model verification. The accurate prediction of macrosegregation remains a significant challenge, as it requires not only an accurate description of the thermal and flow fields but also requires an accurate description of microsegregation and flow within the developing solid network and/or sedimentation of grains. Of note: the above models were mainly used on primary metal production processes such as DC-casting of aluminum alloy and ingot casting of steel and to the author’s knowledge have not been applied to the low-pressure die casting of automotive parts.

2.3 Porosity Prediction

This section focuses on reviewing previous work reported on hydrogen-based pore nucleation and growth and models that simulate these processes.

2.3.1 Hydrogen-based Pore Nucleation

Due to variation in hydrogen solubility between the solid and liquid phases in aluminum alloys, hydrogen is rejected at the liquid/solid interface resulting in an increase in hydrogen concentration in inter-granular, dendritic liquid, during solidification. In addition, the solubility limit of hydrogen in the liquid decreases with both temperature and pressure[9]. When the local hydrogen concentration, or more precisely the hydrogen partial pressure, surpasses the local
pressure and an amount associated with the creation of surface area, a pore can nucleate, as described below

\[
P_{H_2} = \left( \frac{f_H \cdot \text{wt\%}_H}{K_{SP,H_{Al}}} \right)^2 > P_{local} + \frac{2 \gamma}{r}
\]

where \( f_H \) is the Henrian 1 wt.% activity coefficient of H in Al, \( K_{SP,H_{Al}} \) is the Sieverts’s constant of hydrogen in the liquid and \( P_{local} \) is the local pressure calculated accounting for the metallostatic head and pressure drop associated with flow through the developing solidification microstructure (often estimated using Darcy’s law), \( \gamma \) is the surface tension of the pore liquid interface, \( r \) is the pore radius.

However, the classical homogeneous nucleation theory requires an excess hydrogen activity or pressure on the order of several GPa for nucleation to occur, which is not observed practically. Therefore, it may be concluded that hydrogen porosity generally nucleates heterogeneously on viable substrates that reduce the supersaturation required significantly. Foreign particles like oxide inclusions present in the melt, which are not well wetted by the liquid, can act as potent sites for pore nucleation. Campbell[41] has argued that it would still be quite difficult for hydrogen gas pores to nucleate heterogeneously without entrained oxide bi-films and pointed out that the entrainment of an oxide film is likely to occur during the pouring process.

The exact mechanism, or mechanisms, by which hydrogen pores nucleate is not fully understood. All of the existing models include significant assumptions and empiricism. Poirer et al.[42] developed the following expression to determine if pore nucleation takes place

\[
P_{H_2} - 4 \gamma / (1 - f_l) \lambda_2 \geq P_{local}
\]

where \( f_l \) is solid fraction, \( P_{H_2} \) is the equivalent partial pressure of hydrogen gas in solution and \( P_{local} \) is the local pressure, \( \gamma \) is the surface tension and \( \lambda_2 \) is the secondary dendrite arm spacing.
Application of this relationship suggests pore nucleation would occur at a high fraction of solid, contrary to what has been observed in tests[43]. More recently, a pore nucleation model applying a stochastic method was developed to describe the density of nucleation sites $n_p$ with respect to temperature with a Gaussian function[44]:

\[
\frac{dn_p}{dT} = \frac{n_{\text{max}}}{T_\sigma \sqrt{2\pi}} \exp\left\{-\frac{(T - T_N)^2}{2T_\sigma^2}\right\} \tag{Equation 2.11}
\]

where $n_{\text{max}}$ is the maximum number of nuclei, $T_\sigma$ and $T_N$ are the deviation and the mean temperature of the Gaussian function. All of the parameters are expected to vary with cooling rate and can be derived by a least-squares fitting method. In a subsequent paper, Lee[45] linked the nucleation temperature in the Gaussian function to hydrogen supersaturation, which was defined as the ratio of local hydrogen concentration to the solubility of hydrogen in the liquid. The local hydrogen concentration was calculated based on lever rule. The solubility of hydrogen in the liquid was presented in the form of van’t Hoff equation using an approach outlined in paper by Poirier et al. [42]. It was found that micropores nucleated when the hydrogen supersaturation reached a level around 2.0 with a standard deviation of 0.5. Recently, Yao et al. [46] adopted a different approach from Lee[45] to express the hydrogen supersaturation ($mol/m^3$). In this work, hydrogen supersaturation was defined as the difference between the local hydrogen concentration and the critical hydrogen concentration. By applying above definition, the potential effects of hydrogen macrosegregation via local hydrogen concentration and pressure drop via the critical hydrogen concentration on pore nucleation can be taken into account. In the reference[46], the distribution of the heterogeneous nucleation sites was related to the melt properties (population and effectiveness of entrained oxides), as shown in Equation 2.12:
\[
\frac{dN_{\text{nuc}}}{dss} = \frac{A}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(ss-ss_0)^2}{2\sigma^2}\right)
\]  

Equation 2.12

where \(N_{\text{nuc}}(\text{mm}^{-3})\) is the number density of the nuclei, and \(A(\text{mm}^{-3}), ss_0(\text{mol/m}^3)\) and \(\sigma(\text{mol/m}^3)\) are determined by fitting with experimental data, which are dependent on the melt properties not on the hydrogen concentration in the melt.

### 2.3.2 Hydrogen-based Pore Growth

In a study by Atwood et al. [45], it was found that the pressure drop in the mushy zone is too small to have an effect on pore size under the Bridgman-typed casting conditions in their work. They developed a model where pore growth is controlled by the rate of hydrogen diffusion to the pore-liquid interface. This concept was extended in [46] and [47], and illustrated in Figure 2.7.

![Diagram of gas component diffusion into a pore (a) and concentration profile in an ideal spherical geometry (b)](image)

**Figure 2.7** Schematics about gas component diffusion into a pore (a) and concentration profile in an ideal spherical geometry (b)[9]

where \(C_{g_l}\) and \(C_{g0}\) are the gas concentration at the liquid-pore interface and in the bulk liquid respectively; \(R_p\) and \(R_{p0}\) are pore radius and solute depletion radius. As shown in Figure 2.7(b), the pore is assumed to form initially as a sphere in the liquid with a radius of \(R_p\). The flux of hydrogen at the pore-liquid interface can be estimated and used to predict the evolution in the pore size with time, as shown below[9]:

23
where $C_{H,L}$ is the hydrogen concentration in the liquid; $\rho_L$ is liquid density; $M_H$ and $N_H$ are molar mass and mole of hydrogen element (for Hydrogen, $M_H N_H = M_{H_2} = 2$); $R$ is the gas constant, $V_p$ and $P_p$ are pore volume and pressure, respectively. Applying $P_p = P_l + 2 \gamma_l / R_p$ and $V_p = \frac{4}{3} \pi R_p^3$ into Equation 2.13, the change in pore size as a function of time can be obtained.

### 2.3.3 Microporosity Models

So far, the approaches proposed for modelling microporosity formation can be categorized into three types\[11\]: (i) analytical solutions; (ii) criteria models based upon empirical functions; and (iii) numerical models incorporating one or more phenomena including nucleation and diffusion controlled pore growth model. For the sake of brevity, only the key numerical models are presented below.

The most straightforward microporosity numerical simulation was a deterministic-type (DE) model\[45\], where pores with uniform size were assumed to be distributed equally throughout an Al-7wt.%Si alloy casting and the growth of each pore was explicit tracked. The DE model did not include nucleation processes, as all of the pores were assumed to nucleate instantaneously. The DE model focused on pore evolution in the radial direction, due to hydrogen diffusion, under the assumption that the pores remain as spheres. The model was solved numerically in the following sequence: first, the gas pressure within the pore, hydrogen equilibrium solubility and number of pores were calculated for a given initial temperature and pore size. Then, the solid fraction and silicon concentration in the liquid for each subsequent time step were calculated using the Scheil equation. Hydrogen solubility was updated as a function of temperature, and the pressure change
and the hydrogen distribution was updated by solving the bulk transport equation. The DE-type models provided a prediction of the final average pore radius ($\mu m$) and percentage porosity ($\%$).

In order to overcome the limitation on pore nucleation found in the DE-type models, Felicelli et al. [48] introduced pseudo-solutes into the system to represent potential nucleation sites. The distribution of pseudo-solutes during solidification was then obtained by solving fluid momentum equations at the macro scale. Whether or not a pore nucleates on pseudo-solutes is determined by applying Equation 2.10. In [48], both the pore radius and the number of pseudo-solutes were assumed and specified as initial conditions. The proposed model was applied to predict average pore radius ($\mu m$) and percentage porosity ($\%$) in aluminum A356, which was treated as a quaternary alloy (Al-Si-Mg-H) solution. The simulated results with various initial hydrogen concentrations were in good agreement with experimental results. However, the model did not indicate stochastic nature of pore nucleation. Lee [44] included this feature by developing a continuum stochastic (CS) model, where hydrogen conservation equation was solved through a finite difference (FD) algorithm. Initially, a random distribution of potential nuclei was chosen, although other distributions of potential nuclei sites could also be used [36]. Once the hydrogen concentration exceeded the degree of supersaturation, defined as a pore nucleation temperature, pores would nucleate on the activated nuclei. The simulation results were in good agreement with experimental results in terms of pore radius and pore density. Further experimental work, using a Temperature Gradient Stage coupled with X-ray radiography revealed a discrepancy between the CS model and the X-ray based measurement [36] in terms of pore growth. One possible explanation for this discrepancy was that the model did not consider the effect of the development of solid microstructure on porosity formation.
To consider the interaction of pore growth with microstructure, Rappaz et al.\[49\] proposed the use of a cellular automata (CA) method. In CA, the state of each computational cell in the coupled model can be either liquid, solid or mushy. In addition, all three states can possess pores. The combination of CA model and CS model enable simultaneous simulation of nucleation and growth of both the solid phase and porosity based on local undercooling and degree of supersaturation. A similar treatment to CS models was adopted for hydrogen diffusion. However, the pore growth process was treated slightly differently between these two models. Pore growth was confined to a single cell in CA model, whilst pore was allowed to grow into neighbouring cells in CS model. Thus, compared to CS model, CA model produced smaller pores but in greater number. Although the CA model improved the accuracy of pore growth rate and integrated most of the complex physical phenomenon, it required a smaller mesh and was computationally intensive, making it hard to be applied to real industrial situations. Recently, Zhu et al.\[50\] proposed a 2-D CA-FDM (finite difference method) model to simultaneously simulate the solid microstructure and porosity distribution during solidification of Al-7wt.%Si. The CA method was adopted to simulate the growth of the dendrites and pores while the FDM method was used to simulate the diffusion of solute and hydrogen. The proposed model included hydrogen partitioning, nucleation of porosity and the competitive growth of both the dendrites and pores. The model was validated by comparing the predicted pore volume fraction against the measurement data in the literature. Although the model showed relatively good agreement and could evaluate the effects of hydrogen content, the model was developed for a relatively small domain and ignored the effect of fluid flow on the evolution of solute concentration in the liquid.

Recently, Yao et al.\[46\] developed a numerical model to predict the pore size distribution for hydrogen-based microporosity. Similar to the CS model, a Gaussian function was adopted to
quantify the distribution of the heterogeneous pore nucleation sites. The authors applied a similar approach to [45] in order to simulate diffusion-limited pore growth, however, they also added the effect of microstructure on pore growth. Finally, a binning method was applied to track the growth of a group of pores nucleated within a given range in supersaturation, instead of tracking the nucleation and growth of individual pores. The porosity model was implemented through a FORTRAN program and the evolution of temperature and pressure at specific locations were calculated through CFD commercial package Ansys-CFX 12.0. The predictive capability was evaluated by comparing against directionally solidified A356 alloy specimens with the pore volume fraction and size distribution measured using X-ray microtomography (XMT). The simulation results and experimental results were in good agreement in terms of pore volume fraction and size distribution. Although the proposed model could evaluate the effects of hydrogen content, cooling conditions and degassing time on microporosity formation, the effect of macro-segregation of hydrogen on microporosity formation was not included. In addition, under the directional solidification conditions used in the experiments for model validation, there was a limited pressure drop needed to feed solidification shrinkage. Thus, the role of an inter-dendritic drop in pressure was not assessed.

Most recently, Gao et al.[51] proposed a theoretical model to couple porosity formation and solute segregation behaviour in the interdendritic liquid during directional solidification of Al-Cu alloy. The author pointed out that enrichment in alloying constituent could be reduced as a result of the presence of porosity, which partly compensates for solidification shrinkage leading to a reduction in flow rate of the enriched liquid.
3 Project Objectives and Scope

Objective - Microporosity can act as fatigue crack initiation sites in castings subject to cyclic loading depending on pore size and whether or not an individual, or clusters, of pores are located in an area of high cyclic stress. Consequently, and as described in the literature review, there has been a sustained effort over a number of years to develop computational models that predict pore formation, particularly in aluminum alloys since they are prone to the formation of hydrogen-based microporosity. However, one aspect of micro-pore formation that has not been considered previously in detail is the effect of macro-segregation of both hydrogen and solute species affecting solidification. This research will focus on the numerical simulation of hydrogen and silicon macrosegregation during solidification of A356 and its impact on hydrogen-based pore formation. The objective of the work is to develop a robust pore formation model suitable for application to the low pressure die casting of automotive wheels.

Scope - To meet the overall program objective the following sub-tasks were completed:

1. To begin, a simple axisymmetric A356 casting with an L-shaped profile was developed, since it shares similar geometric features to the rim/spoke of a cast automotive wheel.

2. Using the geometrically simplified model, a user-defined function was formulated to solve for both silicon segregation and hydrogen segregation. Note: ANSYS-FLUENT has a built-in capability to predict micro and macro-segregation of major alloy species, such as silicon, but not hydrogen. As a means of verifying the formulation of the user-defined function, the silicon concentration variation predicted using the function was compared with the variation predicted using the built-in capabilities of the code.
3. Once verified, a sensitivity analysis was conducted using the geometrically simplified model to assess the impact of some of the assumptions made in developing the user-defined function as well as some of the numerical implementation/control options adopted for execution of the code.

4. The focus was then shifted to developing the model of the low-pressure die casting process. Following development, this model was validated against a combination of thermocouple data collected from the industrial process and silicon segregation data extracted from a commercially produced wheel.

5. Finally, the fully coupled thermal-fluid-species model was used to output the evolution in temperature, fraction liquid/solid, and pressure and hydrogen concentration at points of interest in the wheel during solidification. This information was then input to the hydrogen-based pore formation model based on one previously developed at UBC, which is capable of predicting the size distribution of hydrogen-based pores in A356[46]. Using this approach, the nucleation and growth of pores are tied to the local pressure, fraction liquid and concentration of hydrogen (accounting for macrosegregation associated with shrinkage-induced flow), in a sequentially coupled manner. The predicted results from the porosity model were then compared against measurements of the pore size distribution obtained from a production wheel using x-ray microtomography.

A schematic of the overall modelling methodology and flow of data is shown in Figure 3.1.
Figure 3.1 Schematic of the overall modelling methodology used to predict pore size distribution for L-shaped and LDPC casting
4 Model Development

A coupled thermal-fluid-composition model has been developed using the commercial CFD software package, FLUENT, version 16.0. FLUENT adopts the finite volume method (FVM) to solve for the conservation equations (momentum, energy and species) over finite volumes. The first step in the FVM is to discretize the computational domain into non-overlapping finite volumes, and the unknown variables are evaluated at the centroids of the volume elements. The solutions of each unknown variable are obtained through the volume integral of the partial differential equations over the finite volume. The FVM technique is inherently conservative and can provide quick analysis on a complex system with unstructured meshes and various boundary conditions[52]. These characteristics have made FLUENT suitable for the numerical simulation of a solidification process, which involves fluid flow, heat and species transfer.

FLUENT contains a basic solidification module along with an open architecture that permits additional functionality to be added via user-defined subroutines. As previously described, the objective of the project is to examine the role of silicon and hydrogen macrosegregation on hydrogen-based pore formation. Macrosegregation of silicon can be predicted using the built-in capabilities of the code. The first challenge encountered is how to account for hydrogen segregation. Hydrogen cannot directly be introduced as an additional alloy constitute, as the code is formulated to account for the effect of normal alloy additions on the liquidus and solidus temperatures, using a pseudo binary approach. In the pseudo binary approach, the slope of the liquidus temperature is extracted from their respective binary phase diagrams and then their effect on the alloy is accounted for using a weighted average approach. In the case of hydrogen, it does not affect the liquidus temperature nor does it form a eutectic. This issue was addressed by
developing a user-defined scalar (UDS) in FLUENT to describe the conservation of hydrogen, accounting for bulk transport.

In this chapter, section 4.1 and 4.2 focus on the techniques used in FLUENT to solve the transport equations in the context of a solidification problem. Following that, section 4.3 briefly introduces the porosity model to predict the pore size distribution. Then, section 4.4, provides a detailed description of a prototype model, which was used to validate the proposed UDS method. A series of sensitivity analysis were undertaken in section 4.5. Section 4.6 elaborates the updates to the original porosity model[46].Section 4.7 shows the application of the porosity model to predict pore size distribution and porosity fraction at a key location for species enrichment found in the prototype model. A series of sensitivity analysis regarding the updated porosity model were undertaken in the last section 4.8.

4.1 Description of The Methodology for Numerical Simulation

Solidification is a phase transformation process, dominated by heat transfer, but also dependent on species transport phenomena. In FLUENT, the solidification module is developed based on binary solidification systems. The enthalpy-permeability approach[32] is applied to simulate the transport phenomena in the mushy zone (two-phase zone) which is treated as a porous medium. The solid/liquid interface is not tracked explicitly during the solidification process. Instead, a variable called the liquid volume fraction, \( f_l \), is introduced and calculated at each cell in the domain. The liquid fraction quantity in each cell varies from 0 to 1 to represent the phase of each cell – i.e. completely solid \( (f_l = 0) \), a mixture of solid and liquid \( (0 < f_l < 1) \) and completely liquid \( (f_l = 1) \). Significant phenomena during solidification, such as the release of latent heat, the variation in permeability in the two-phase, or mushy, zone and amount of solute rejected from the
solid to the liquid (normally segregating species with a segregation, or distribution, coefficient, \( k_i < 1 \)) are all directly associated with liquid fraction. The generic form of the governing equations related to the solidification process is given as[32] :

\[
\frac{\partial (\rho \phi)}{\partial t} + \nabla \left( \rho \vec{v} \phi \right) = \nabla \left( \Gamma \nabla \phi \right) + S
\]

Equation 4.1

in which, \( \rho \) (kg/m\(^3\)) is the density, \( \vec{v} \) (m/s) is the velocity of the fluid, \( \phi \) represents the conserved property (energy, momentum, species concentration), \( \Gamma \) represents the diffusion coefficient and \( S \) is the source term. The terms on the left-hand side of Equation 4.1 represent the accumulation term and the advection term, respectively. The first term on the right-hand side of Equation 4.1 represents the diffusion term. A detailed description is given below with respect to each governing equation (mass, momentum, energy and species conservation) used in the FLUENT solidification module for the current work.

4.1.1 Mass Continuity Equation

Mass continuity states that the rate at which mass is accumulated in the system is equal to the amount at which mass enters the system, minus the amount that leaves the system. Assuming that mass is neither lost nor gained from/by the system, the mass fraction \( \phi \) can be set to 1 throughout the domain. Also, since there is no gradient in mass fraction and sources or sinks of mass, the two terms on the right-hand-side of Equation 4.1, can be set to 0. The mass conservation equation for a representative volume element (RVE) or computational cell becomes:

\[
\frac{\partial (\rho)}{\partial t} + \nabla \left( \rho \vec{v} \right) = 0
\]

Equation 4.2

Note: that the FLUENT solidification module treats the liquid, two-phase mushy zone and solid as a single phase. Thus FLUENT does not permit consideration of the hydrogen gas in the continuity equation. Thus, the effect of gas evolution on the need to supply mass in the mushy
zone to compensate for solidification shrinkage is not accounted for in FLUENT. Since the volume of hydrogen-based porosity formed in the LPDC process for wheels is small compared to the liquid-to-solid volume change, it is reasonable to neglect the presence of the gas phase and its effect on shrinkage driven flow.

Following on from this assumption, the average density $\rho$ in the mushy zone is defined as: $\rho = \rho_i f_i + \rho_s f_s$, where $\rho_i$ is the density for each phase ($i = l$ for liquid, $i = s$ for solid). Further, assuming that there is adequate liquid feeding and volume is conserved, the sum of the volume fractions of each phase satisfies the expression, $f_l + f_s = 1$. It follows that the mass flux term $\nabla \left( \rho \vec{v} \right)$ can be defined as $\nabla \left( \rho \vec{v} \right) = \nabla \left( \rho_l f_l \vec{v}_l + \rho_s f_s \vec{v}_s \right)$, where $\vec{v}$ ($m/s$) is the velocity for each phase. Therefore, the mass conservation equation can be re-rewritten in the following form:

$$\frac{\partial (\rho)}{\partial t} + \nabla \left( \rho_l f_l \vec{v}_l + \rho_s f_s \vec{v}_s \right) = 0$$  \hspace{1cm} \text{Equation 4.3}

The term $\left( \frac{\partial \rho}{\partial t} \right)$ in Equation 4.3 represents density change upon solidification. This represents the general case, in which, solidification shrinkage due to a density variation may be compensated by either liquid flow $\nabla \left( \rho_l f_l \vec{v}_l \right)$ and/or solid movement $\nabla \left( \rho_s f_s \vec{v}_s \right)$ - e.g. tension, compression or settling. As the solid phase is assumed to be fixed in the current work, the contribution from solid motion can be ignored. The mass conservation equation is reduced to:

$$\frac{\partial (\rho)}{\partial t} + \nabla \left( \rho_l f_l \vec{v}_l \right) = 0$$  \hspace{1cm} \text{Equation 4.4}

In summary, the solidification shrinkage in the current work is assumed to be compensated by liquid feeding exclusively. The correction in the mass conservation equation needed when
encapsulation occurs – i.e. mass feeding ends – and significant shrinkage porosity develops is not considered in the current analysis.

4.1.2 Momentum Conservation Equation

In terms of momentum conservation equation, which is based on Newton’s second law, \( \phi \) is set to velocity \( \vec{v} \) \((m/s)\) and \( \Gamma \) is set to liquid viscosity, \( \mu \) \((Pa\ s)\). In FLUENT, a momentum source term, \( S \) \((kg/m^2/s^2)\), as described below, can be added to represent the momentum resistance as the permeability reduces in the mushy zone[53]:

\[
s = -\frac{(1 - f_i)^2}{\left(f_i^3 + \epsilon \right)} A_{mush} \vec{v} \tag{Equation 4.5}
\]

where \( \epsilon \) is a small number (0.001) added to avoid division by zero (This is specified by FLUENT and cannot be altered). \( \vec{v} \) is the superficial liquid velocity, equal to the product of liquid fraction and liquid velocity, \( \vec{v} = f_i \vec{v}_l \). \( A_{mush} \) \((kg/m^3.s)\) represents the amplitude of velocity attenuation, the higher the value, the steeper the reduction of the velocity of the liquid phase as \( f_i \) becomes zero. Equation 4.5 can be derived from Darcy equation, which is routinely applied to solve for the velocity or pressure drop associated with flow through porous media. The correlation[9] between liquid velocity and pressure drop can be expressed as:

\[
f_i \vec{v}_l = -\frac{K}{\mu} (\nabla P - \rho_l g) \tag{Equation 4.6}
\]

where \( K \) is the permeability, \( \mu \) \((Pa\ s)\) is the liquid viscosity , \( P \) \((Pa)\) is the pressure and \( g \) is the gravity vector. The permeability, \( K \), has been estimated based on Equation 4.7, the so-called Carman-Kozeny equation, for flow through a packed bed of spheres and is the most widely used correlation for solidifying systems.
where $\lambda_2 (\mu m)$ is the secondary dendrite arm spacing (SDAS). Combining Equation 4.6 and Equation 4.7 gives

$$K = \frac{\lambda_2^2}{180} \frac{f_i^3}{(1 - f_i)^2}$$  \hspace{1cm} \text{Equation 4.7}[47]$$

The right-hand side of Equation 4.8 represents the reduced force per unit volume ($kg/m^2/s^2$) or reduced momentum. Thus, the left-hand side of Equation 4.8 is the same as Equation 4.5. By comparison, $A_{\text{mush}} = \frac{180 \mu}{\lambda_2}$ and is a function of the liquid viscosity and the secondary dendrite arm spacing (SDAS). SDAS can be estimated through the local cooling rate by an experimentally derived correlation[54]. Figure 4.1 shows the variation of $A_{\text{mush}} (kg/m^3s)$ with SDAS, assuming a liquid viscosity of 0.0014 $kg/m/s$.

![Figure 4.1 Variation of $A_{\text{mush}} (kg/m^3s)$ with respect to SDAS (\mu m) assuming a constant liquid viscosity of (0.0014 $kg/m/s$)](image-url)
For instance, when the size of SDAS is 50 $\mu m$, the computed $A_{mush} \text{ (kg/m}^3\text{s)}$ is around $10^8$ whereas the default value of $A_{mush} \text{ (kg/m}^3\text{s)}$ in FLUENT is $10^5$. Since the SDAS depended $A_{mush} \text{ (kg/m}^3\text{s)}$ may cause the numerical solution to oscillate, $A_{mush} \text{ (kg/m}^3\text{s)}$ is set to a constant. The effect of $A_{mush} \text{ (kg/m}^3\text{s)}$ on the evolution of pressure and velocity will be discussed later in this chapter.

### 4.1.3 Energy Conservation Equation

In terms of the energy conservation equation, $\phi$ is set to enthalpy $H \text{ (J/kg)}$ in the accumulation term and advection term. $\Gamma$ is set to the conductivity of the material $k \text{ (W/m} K)$ in the diffusion term. The resulting expression is shown in Equation 4.9,

$$\frac{\partial (\rho H)}{\partial t} + \nabla \left( \rho \nu H \right) = \nabla (k \nabla T) + S$$

Equation 4.9

where $S \text{ (J/m}^3\text{s)}$ is a source term and the enthalpy of the material $H \text{ (J/kg)}$ in FLUENT is given as:

$$H = h_{ref} + \int_{T_{ref}}^T C_p dT + f_i L$$

Equation 4.10

where $h_{ref} \text{ (J/kg)}$ is the arbitrary reference enthalpy (0 J/kg), $T_{ref} \text{ (K)}$ is arbitrary reference temperature (288.16°K) and $L \text{ (J/kg)}$ is the latent heat. Note: that the source term is set to zero as the latent heat of solidification is embedded in the enthalpy expression. The release of the latent heat is dependent on the evolution of the liquid fraction $f_i$. The evolution in temperature in the material during solidification can be computed by integration of Equation 4.9. Smoothly updating the liquid fraction $f_i$ is the key to yielding a stable solution to the energy equation. Note: that sudden change in $f_i$ - i.e. eutectic phase transformation, may cause convergence issues. Thus, in FLUENT, the method[55] suggested by Voller and Swaminathan is used to update the liquid fraction so as to avoid numerical issues. Please refer to above reference for more details.
4.1.4 Species Conservation Equation

For the species conservation equation, $\phi$ is set to species concentration $C_i$ in the unit of mass fraction and $\Gamma$ is set to the species diffusion coefficient $D_i \ (m^2/s)$. The source term is evaluated based on solute partitioning mechanisms. In the current work, the Scheil model is selected to account for solute redistribution at the scale of the microstructure. Thus, the source term[32] takes the following form:

$$S = -k_i C_{i,\text{liq}} \frac{\partial}{\partial t} \left( \rho (1 - f_i) \right) + \frac{\partial}{\partial t} \left( \rho (1 - f_i) C_{i,\text{liq}} \right)$$

Equation 4.11

where $k_i$ is the partition coefficient of species $i$, $C_{i,\text{liq}}$ is the mass fraction of species $i$ in the liquid. The readers are referred to [32] for the detailed derivation of the source term. The first term on the RHS of Equation 4.11 represents the increase in solute concentration in the solid due to new solid formation. The second term on the RHS of Equation 4.11 represents the increase in solute concentration in the liquid due to solute rejection from growing solid to the liquid. In FLUENT, the species conservation equation first is solved for the species mass fraction in the liquid, $C_{i,\text{liq}}$, and then the overall mass fraction, $C_i$, in both liquid and solid phase. The species conservation equation is expressed as:

$$\frac{\partial (\rho C_{i,\text{liq}})}{\partial t} + \nabla \left( \rho f_i \nu_i C_{i,\text{liq}} \right) = \nabla \left( \rho f_i D_{i,\text{liq}} \nabla C_{i,\text{liq}} \right) - k_i C_{i,\text{liq}} \frac{\partial (\rho (1 - f_i))}{\partial t} + \frac{\partial (\rho (1 - f_i) C_{i,\text{liq}})}{\partial t}$$

Equation 4.12

The first and second terms on the left-hand side of Equation 4.12 represent the accumulation and advection terms respectively. The advection term is responsible for the transfer of solute out of the grain envelope and is one of the well-established mechanisms for the formation of macrosegregation. The first term on the right-hand side of Equation 4.12 represents the diffusion term, which is assumed to be negligible for current work. This has been assessed using the solutal Péclet number, given in Equation 4.13:
\[ P_e = \frac{v_j}{D_{i,liq} / L} \]  

Equation 4.13

where \( v_j \) (m/s) is the velocity of the fluid \( D_{i,liq} \) (m\(^2\)/s) is the diffusion coefficient of species \( i \) in the liquid, \( L \) is the characteristic length. Given that the mass conservation expressions in FLUENT are developed on an element-by-element basis, the characteristic length is assumed to be the mesh size (1 to 5mm). For instance, the velocity of the fluid is around \( 3 \times 10^{-3} \) m/s, mesh size is 1mm and \( D_{H,liq} \) is \( 3 \times 10^{-7} \) m\(^2\)/s and \( D_{Si,liq} \) is \( 4.75 \times 10^{-9} \) m\(^2\)/s, respectively. Therefore, the solutal Péclet number is much greater than 1 for both hydrogen and silicon. As a result, the diffusion term can be ignored in the species conservation equation for macrosegregation. Thus, the species conservation equation can be reduced to:

\[
\frac{\partial (\rho C_{i,liq})}{\partial t} + \nabla \left( \rho_i f_i v_i C_{i,liq} \right) = -k_i C_{i,liq} \frac{\partial (\rho (1 - f_i))}{\partial t} + \frac{\partial (\rho (1 - f_i) C_{i,liq})}{\partial t} \]

Equation 4.14

The overall species concentration, \( C_i \), in each cell is obtained via the following expression\[32\]:

\[
\rho C_i = \rho_i f_i C_{i,liq} + \rho_i \int_{f_i}^{f_i} C_{i,sol} df_i
\]

Equation 4.15

The second term on the right-hand side of Equation 4.15 is required to account for the continuously evolving concentration of the solid at the S/L interface when the concentration in the solid is not uniform.

The variation in the solidus and liquidus temperature with species segregation is also accounted for in FLUENT and can be calculated by Equation 4.16 and Equation 4.17 as follows:

\[
T_{solidus} = T_{melt} + \sum_{solutes} m_i C_i / k_i \]

Equation 4.16

\[
T_{liquidus} = T_{melt} + \sum_{solutes} m_i C_i
\]

Equation 4.17

where, \( m_i \) (K/wt.%) is the slope of liquidus line with respect to species \( i \), \( C_i \) is the overall mass fraction of species \( i \) and \( k_i \) is partition coefficient of species \( i \). As soon as temperature drops
below $T_{liquidus}$, solidification occurs. This approach assumes that the contribution of various species to update the liquidus temperature is additive based on the individual binary alloy phase diagrams. 

*Note: if input $C_i$ is larger than the eutectic mass fraction of species $i$, then $C_{i,Eut}$ is used to calculate liquidus and solidus temperatures.*

### 4.2 Hydrogen Species Conservation

As previously described, one of the goals of the research program was to calculate the macrosegregation of hydrogen and to link the local hydrogen concentration to pore formation using a pore nucleation and growth model, previously developed at UBC. Referring to the species conservation equations presented in Section 4.1.4, FLUENT’s default solidification modelling capabilities allow for prediction of the local concentration of alloying species in the liquid phase and the overall alloy concentration, see Equation 4.14 and Equation 4.15, accounting for bulk transport outside of the gain envelope. Unfortunately, it does not allow for the tracking of non-alloying species such as hydrogen (Note: the introduction of hydrogen tracking using the built-in capabilities would require inputs of the eutectic mass fraction of hydrogen and the slope of liquidus line of the Al-H system. Practically speaking, there is not a “eutectic” in the Al-H system, and from Al-H phase diagram[56], the presence of hydrogen has no impact on the melting (liquidus) temperature of aluminum).

In order to avoid assigning fictitious values for these quantities during model development, which could have unintended consequences, hydrogen was introduced into the system as a user-defined scalar (UDS in FLUENT’s nomenclature), which is evaluated in user-defined functions (UDFs in FLUENT’s nomenclature).
In FLUENT, the species conversation equation first is solved for the species mass fraction in the liquid, \( C_{i,\text{liq}} \), and then the overall mass fraction, \( C_i \), in both liquid and solid phase. Thus, two user-defined scalars are required to solve for hydrogen macrosegregation. \( UDS_0 \) and \( UDS_i \), respectively, represent the hydrogen mass fraction in the liquid and overall mass fraction of hydrogen. Replacing \( C_{i,\text{liq}} \) with \( UDS_0 \) in Equation 4.14 leads to:

\[
\frac{\partial(\rho UDS_0)}{\partial t} + \nabla \left( \rho_f f_i \nu_i UDS_0 \right) = -k UDS_0 \frac{\partial (1-f_i)}{\partial t} + \frac{\partial (\rho (1-f_i) UDS_0)}{\partial t} \quad \text{Equation 4.18}
\]

Once \( UDS_0 \) is solved through Equation 4.17, the overall mass fraction of hydrogen (\( UDS_i \)) can be computed from:

\[
\frac{\partial}{\partial t} (\rho UDS_i) = \frac{\partial}{\partial t} (\rho_f UDS_0) + k UDS_0 \frac{\partial}{\partial t} (\rho (1-f_i)) \quad \text{Equation 4.19}
\]

The readers are referred to [32] for detailed derivation of Equation 4.18. The user-defined functions (UDFs) are implemented to solve for above functions.

### 4.3 Porosity Model

As described in Chapter 3, a sequentially coupled in-house porosity model will be used to predict the pore size distribution at several discrete locations in the low-pressure die cast A356 wheel. The porosity model was previously developed by Yao et al. [46]. The porosity model describes both pore nucleation and pore growth. Regarding nucleation, the distribution of the heterogeneous nucleation sites is assumed to be a function of supersaturation \( ss \) (\( \text{mol/m}^3 \)) and can be described by a Gaussian function of the form:

\[
\frac{dN_{\text{nuc}}}{dss} = \frac{A}{\sqrt{2\pi}\sigma} \exp \left( -\frac{(ss-ss_0)^2}{2\sigma^2} \right) \quad \text{Equation 4.20}
\]
where \( N_{\text{nc}} \) (\( \text{mm}^3 \)) is the number density of the nuclei, \( A \) (\( \text{mm}^3 \)) represents total available nuclei, which depends on the inclusion level, such as the number of oxides in the melt, \( \sigma \) (\( \text{mol/m}^3 \)) represents the variation in potency of nucleation sites and \( ss_0 \) (\( \text{mol/m}^3 \)) represents the average supersaturation for pore nucleation. \( A, ss_0 \) and \( \sigma \) are adjustable parameters and associated with the melt properties. The supersaturation \( ss \) (\( \text{mol/m}^3 \)) is defined as the difference between local hydrogen content in the liquid, \( C_{H,\text{liq}} \) (\( \text{mol/m}^3 \)) and the critical local, saturation, concentration \( C_i^e \) (\( \text{mol/m}^3 \)), computed by FLUENT and Sievert’s Law, respectively, where the expression for \( C_i^e \) is given below:

\[
C_i^e = K_L \sqrt{P_a + P_h + \Delta P_d}
\]

Equation 4.21

In Equation 4.21, \( K_L \) [57] is the equilibrium constant (\( \text{mol/m}^3/\text{atm}^{1/2} \)), which is a function of temperature (\( K \)), \( P_o \) (\( \text{Pa} \)) is the atmospheric pressure, \( P_h \) (\( \text{Pa} \)) is the metallostatic pressure, \( \Delta P_d \) (\( \text{Pa} \)) is the pressure drop associated with attenuated flow in the mushy zone (Darcy source term). Note that the output \( C_{H,\text{liq}} \) from FLUENT is in the units of weight percentage. Thus, the nucleation rate is determined by a combination of the characteristics of the melt (number of heterogeneous nucleation sites), local hydrogen concentration and local pressure. Once nucleation occurs, the growth rate of a pore is controlled by the total moles of hydrogen diffusing from the bulk to the pore/liquid interface. The hydrogen mass flux is estimated via the following expression:

\[
\frac{dn_H}{dt} = D_{H,\text{liq}} \cdot 4\pi r_p^2 \cdot \varphi \frac{C_{H,\text{liq}} - C_{lp}}{l_{\text{diff}}}
\]

Equation 4.22

where \( n_H \) (\( \text{mol} \)) is the total moles of hydrogen, \( D_{H,\text{liq}} \) (\( \text{m}^2/\text{s} \)) is the diffusivity of hydrogen in the liquid, \( r_p \) (\( \text{m} \)) is the pore radius, \( \varphi \) is the growth impingement factor, \( (1-f_s)^m \), accounting for the interaction between dendrite structure and the pores, \( m \) is a parameter determined by fitting with
experimental data and \( l_{\text{diff}} \) is the diffusion length in the liquid approximated as the pore radius. The \( C_{lp} \) (mol/m\(^3\)) represents hydrogen concentration at the liquid and pore interface, given by:

\[
C_{lp} = K_L \sqrt{P_a + P_h + \Delta P_d + \frac{2\gamma}{r_p}}
\]

Equation 4.23

Same as Equation 4.21, \( K_L \) [57] is the equilibrium constant (mol/m\(^3\)/atm\(^{1/2}\)) as a function of temperature (K) and \( P_a \) (Pa) is the atmospheric pressure, \( P_h \) (Pa) is the metallostatic pressure, \( \Delta P_d \) (Pa) is the pressure drop associated with Darcy source term and \( \frac{2\gamma}{r_p} \) (Pa) is the pressure exerted by the surface tension. The porosity volume is updated through the ideal gas law as below:

\[
\frac{dn_H}{dt} = \frac{d(P_s V_s / R_s T)}{dt}
\]

Equation 4.24

where \( P_s = P_a + P_h + \Delta P_d + \frac{2\gamma}{r_p} \). It should be noted that \( \Delta P_d \) is one of the driving forces for pore growth and a significant pressure drop during the last stages of solidification can lead to an increase in pore size. The readers are referred to reference[46] for a more detailed description of the porosity model.

### 4.4 Simplified Model of L-Shaped Cross-section Casting of A356

As a precursor to developing 3-D numerical model of the low-pressure die casting process, a 2-D, axisymmetric, L-shaped casting of a binary Al-7wt.%Si alloy was developed. The primary purpose of this geometrically simplified model was to investigate the capability of the solidification module in FLUENT using a computationally less intensive model and also to validate the user-defined functions for predicting hydrogen segregation.

**Computational Domain**
The geometry, mesh and boundary conditions used in the model are shown in Figure 4.2. The domain is meshed using rectangular elements only. The quadrilateral mesh is uniform with a size of 1\text{mm} by 1\text{mm}. The total length and height of the domain are 80\text{mm} and 75\text{mm}, respectively. The number of elements (cells) in the domain is 2205 and the number of nodes is 2376. This specific geometry was selected to be analogous to a basic automotive wheel – see the various subsections that have been labelled with names representing the various components of an actual wheel casting.

**Boundary and Initial Conditions**

The boundary conditions were also simplified, but have been selected to produce solidification conditions similar to that observed in the production of an actual wheel – e.g. a reduced heat transfer coefficient of 1500\text{W/m}^2\text{K} was applied to the sides of the spoke and an
increased heat transfer coefficient of $2000 \text{W/m}^2\text{K}$ to the vertical sides of the rim, whereas an adiabatic boundary condition was applied to the top of the rim and hub side (apart from the symmetry boundary). The top of the hub is defined as a pressure-inlet boundary. Material enters with the same temperature and solute content as the material in the wheel directly adjacent to the boundary.

These boundary conditions generate solidification inward (normal to the rim sides) along/down the rim, then across the spoke, with the last material to solidify located at the top of the hub. Note: in some commercial operations solidification can initially occur mid-rim and then proceed both up toward the top of the rim and down toward the bottom of the rim and across the spoke. The top of the rim is often insulated due to the presence of trapped air. From a fluid flow perspective, the top of the hub was defined using a pressure inlet boundary condition, formulated to produce no net heat or species mass transport associated with the material drawn into the domain to feed the volumetric shrinkage associated with solidification. It was assumed that the initial conditions are a uniform temperature of $973.15 \text{K}$ throughout the simulation domain and a uniform composition of $C_{\text{Si,0}} = 7\text{wt.\%}$.

**Material Properties**

The material thermo-physical properties and FLUENT solidification module parameters used in the model are shown in Table 4.1,

<table>
<thead>
<tr>
<th>Properties</th>
<th>Value</th>
<th>Unit</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal conductivity, $k_f$</td>
<td>$f(T)$</td>
<td>$\text{W/mK}$</td>
<td>[58]</td>
</tr>
<tr>
<td>Specific heat, $C_p$</td>
<td>1150</td>
<td>$\text{J/kgK}$</td>
<td>[58]</td>
</tr>
<tr>
<td>Latent Heat, $L$</td>
<td>397500</td>
<td>$\text{J/kg}$</td>
<td>[59]</td>
</tr>
<tr>
<td>Density of solid, $\rho_s$</td>
<td>2685</td>
<td>$\text{kg/m}^3$</td>
<td>[60]</td>
</tr>
<tr>
<td>Density of liquid, $\rho_l$</td>
<td>2540</td>
<td>$\text{kg/m}^3$</td>
<td>[60]</td>
</tr>
</tbody>
</table>
Viscosity of the liquid, \( \mu \) & 0.0014 & kg/m\(s\) & [58] \\
Partition Coefficient of Si, \( k_{Si} \) & 0.13 &  & [61] \\
Eutectic mass fraction of Si & 0.126 &  & [61] \\
Slope of the liquidus, \( m_{Si} \) & -658.73 & K/wt.\% & [61] \\
Melting Temperature of pure Al, \( T_m \) & 933.15 & K & [61] \\

*The properties such as viscosity of the liquid, density of the solid and the liquid are all dependent on temperature, however the model adopted a constant value for the sake of simplicity.*

**Solution Method**

The fully coupled model incorporates the relevant solidification phenomena including mushy zone resistance (Darcy flow damping), latent heat evolution, and solute partitioning during the phase change. The effect of buoyancy-driven flow has been neglected given the limited time the material remains in the liquid state and the presence of relatively small gradients in solute content and temperature in the liquid. The default mushy zone parameter \( A_{mush} \) of 10\(^5\) was applied. Therefore, the only driver for flow is the density change associated with solidification – so-called compensatory flow.

For convergence, the residuals in FLUENT were set to 10\(^{-6}\) for energy, 10\(^{-3}\) for continuity and velocities and 10\(^{-5}\) for species. A fixed time step size of 0.002\(s\) was used. The model took approximately 1 hour to run on 4 Intel(R) Xeon(R) CPUs (2.33GHz).

**Results and Discussion**

To begin, the discussion focusses on the basic fluid flow, solidification and segregation capabilities of FLUENT using silicon as the segregating species. The discussion then moves on to compare the UDF-based prediction of silicon segregation with the built-in capabilities of FLUENT as a means of indirectly validating the formulation of the UDF for hydrogen segregation – e.g. if the formulation for silicon reproduces the results for the built-in prediction, then by similarity, an
identical formulation for hydrogen will also be verified. Finally, a sensitivity analysis is presented using the 2-D L-shaped model.

**FLUENT’S Basic Fluid Flow, Solidification and Segregation Capabilities**

Figure 4.3 shows contours of temperature for the L-shape casting at 5.5, 8.5 and 15s. Black, grey, and white lines have been overlaid on the contour images to mark the positions of the liquidus temperature, (613.8°C, \( f_s =0.0001 \)), \( f_s =0.5 \) and \( f_s =1.0 \), respectively. Based on Al-Si phase diagram, the alloy \( (C_{Si,0} = 7\text{wt.\%}) \) will undergo the eutectic transformation at \( C_{Si,liq} = 12.6\text{wt.\%Si} \), at an \( f_s = \sim 0.5 \) under equilibrium conditions. Note: the evolution of \( f_s \) with temperature is not a unique relationship due to the effect of macrosegregation, which if occurring, can continuously alter the liquid composition as solidification proceeds, beyond that due to microsegregation. The eutectic transformation, which completes solidification, will always occur at \( C_{Si,liq} = 12.6\text{wt.\%Si} \). The approach used by FLUENT to increment the solid fraction with temperature/composition, including after reaching the eutectic composition, is discussed in more detail later in this Chapter.

Returning to Figure 4.3, given the boundary conditions applied in the geometrically simplified casting, solidification starts at the sides of the rim and proceeds inward, then downward along the rim, across the spoke and completes at the hub. At 8.5s, the grey line forms a loop, suggesting the potential exists to encapsulate liquid in the spoke and form shrinkage porosity.
Figure 4.3 Solidification sequence

Figure 4.4 shows contours of velocity magnitude together with velocity vectors at 5.5, 8.5 and 15s. The black, grey and white contour lines have also been included. As shown in Figure 4.4, the liquid is drawn in through the top of the hub (pressure inlet boundary) to supply the volume needed to offset the shrinkage associated with the liquid-to-solid phase transformation. The flow reaches its maximum near the liquidus line (black line) at all three times. Note: the channelling that occurs in the lower part of the rim and in the spoke is due to the increased Darcy resistance as $f_i$ decreases. The effect of velocity attenuation parameter ($A_{mash}(kg/m^3.s)$), used in the Darcy term, on the evolution of velocity magnitude will be investigated later in this Chapter. Comparing velocity magnitudes at the rim/spoke junction (see red circle) at 5.5 and 8.5s, it appears that there is a small area of increased velocity at 8.5s.
Figure 4.4 Velocity magnitude at 5.5, 8.5 and 15s

Figure 4.5 shows contours of pressure (gauge pressure) overlaid with velocity vectors at 5.5, 8.5 and 15s, together with the black, grey and white contour lines. The gauge pressure is measured relative to atmospheric pressure. Thus, 0Pa at a given point in the calculation domain represents the atmospheric, or ambient, pressure. The largest pressure drop, approximately 100Pa (0.001atm), is observed in a large portion of the upper rim at 8.5s and develops as a result of the increased resistance to flow up the channel that forms in the rim. Note: the gradient in pressure that develops at the spoke/rim junction. The evolution of pressure after solidification should be ignored since pressure has no physical meaning in the solid. Note: the absence of a pressure gradient in the upper rim, which suggests a lower bound on the pressure that can be predicted with FLUENT toward the end of solidification at high levels of $f_s$ and flow attenuation.
Figure 4.5 shows contours of the liquid mass fraction of silicon calculated by FLUENT at 5, 8.5 and 15s into the solidification process together with the black, grey and white contour lines. For reference, the initial mass fraction of silicon in the liquid is 0.07. Given the solidification sequence (see Figure 4.3), the liquid phase, in general, becomes enriched with solute as solidification proceeds due to the rejection of solute from the solid, $k_{si} = 0.13$. The evolution in the composition of the liquid will depend on the rate of rejection of solute and rate of transport of solute into or out of the “grid point” due to the bulk motion. The liquid composition using the Scheil model will reach the eutectic composition, irrespective of the initial alloy Si composition. Note: FLUENT outputs and plots the composition of the last liquid present at a given point in the calculation domain, post completion of solidification – see white contour line.

Turning to Figure 4.6, note that there appears to be some entirely solid material with a composition of the last liquid to freeze slightly less than the eutectic composition – see 8.5s at the rim/spoke junction in proximity to the areas of liquid encapsulation in the spoke toward the rim and 15s at the hub/spoke junction. This does not make sense and likely represents a numerical error.
Figure 4.6 Liquid mass fraction of silicon calculated by FLUENT at 5.5, 8.5 and 15s

To further investigate this, the evolution of the solid fraction with temperature and the composition of the liquid with temperature has been output from FLUENT and plotted in Figure 4.7 as a function of $f_s$ at three Points: Point 1, at the top rim; Point 2, at the rim/spoke junction, where liquid encapsulation occurs; and Point 3, in the area that solidifies with the last liquid below the eutectic. The results associated with Point 1 are plotted in red, Point 2, in blue and Point 3, in green. In the upper plot, the black dashed line indicates the equilibrium eutectic temperature, while in the lower plot, the black dashed line shows the results for the Scheil equation.
Turning to the upper plot, there is an inflection point that occurs at all three locations at the eutectic temperature. However, instead of abruptly increasing $f_s$ to 1, FLUENT gradually proceeds to complete solidification over a range of temperature (down to as low as $\sim 555 \, ^\circ\text{C}$ at Point 2). Based on the theory manual, FLUENT increments $f_s$ based on the difference between the local cell temperature, $T$, (as determined from the energy conservation equation) and the equilibrium dendrite tip, or interface, temperature, $T^*$, (as determined from the local species composition, $C_i$). The expression employed is shown in Equation 4.25.
\[ f_{i}^{n+1} = f_{i}^{n} - \lambda \frac{a_{p}(T - T^*) \Delta t}{\rho V_{vol} L - a_{p} \Delta t L \frac{\partial T^*}{\partial f_{i}}} \]  \hspace{1cm} \text{Equation 4.25[53]}

where \( n \) represents increment number, \( \lambda \) is the relaxation factor (default value of 0.9), \( a_{p} \) is the cell matrix coefficient, \( \Delta t \) is the time step size (s), \( V_{vol} \) is cell volume (m\(^3\)), \( T \) is current cell temperature (K) and \( T^* \) is the interface temperature (K). Note: \( T^* \) is calculated from:

\[ T^* = T_{\text{melt}} + \sum_{\text{solutes}} m_{i} C_{i} f_{i}^{k-1} \]  \hspace{1cm} \text{Equation 4.26[53]}

which is the temperature-based form of the Scheil equation, where \( m_{i} \) is the slope of the liquidus of species \( i \), from the binary Al-\( i \) phase diagram and \( C_{i} \) is the composition of species \( i \). The difference between the cell current temperature and interface temperature drives the update of fraction liquid. The derivation of Equation 4.25 is unclear and is claimed to help achieve stability in the solution[55].

The evolution of \( C_{\text{Si,liq}} \) with \( f_{s} \) is dependent on the segregation coefficient and the transport of liquid in to or out of the grain envelope. Irrespective of bulk transport of Si, the eutectic composition should eventually be reached, with the effect being a variation in the \( f_{s} \) at which \( C_{\text{Si,liq}} = 0.126 \) is achieved (and therefore the volume fraction of eutectic). For the Scheil-based evolution (which FLUENT adopts for the source term in the Si conservation equation), \( C_{\text{Si,liq}} = 0.126 \) is achieved at an \( f_{s} \) of approximately 0.5, which would represent the case where there is no bulk transport in or out of the grain envelope. Turning to the lower plot in Figure 4.7, as expected, the evolution of silicon composition in liquid at Point 1 is in good agreement with the Scheil equation since the bulk transport has a negligible effect at this point (see Figure 4.4). The \( C_{\text{Si,liq}} \) at Point 2 is greater than that calculated from Scheil equation at a given \( f_{s} \), suggesting that silicon is enriched locally from bulk transport. In contrast, the \( C_{\text{Si,liq}} \) at Point 3 is less than that calculated from Scheil
equation at a given $f_s$, suggesting that silicon is depleted as a result of bulk transport. Furthermore, at Point 3, $C_{Si,liq}$ reaches peak value at 0.121 at around $f_s = 0.65$, then drops slightly before stabilizing at $C_{Si,liq} = 0.121$ until $f_s = 1.0$, and therefore, does not reach the eutectic composition.

**Verification of User Defined Function (UDF)**

Figure 4.8 through Figure 4.10 compares contours of the User Defined Scalar (UDS), representing the liquid mass fraction of silicon, calculated using the UDF (LHS images) and the liquid mass fraction of silicon calculated with the FLUENT’s built-in capabilities (RHS images) at 5.5, 8.5 and 15s.

![Figure 4.8 Liquid mass fraction of Si obtained through the UDS method (Left) and calculated by FLUENT (Right) at 5.5s](image-url)
Comparing the two sets of images (LHS and RHS), it can be seen that there is a relatively good agreement between the UDF-based concentration of silicon in the liquid and FLUENT-based concentration. Notable differences appear down the centre of the rim, spoke and hub junction and near the hub, which might be associated with the area of encapsulation in the spoke. It is
noteworthy that the UDF-based prediction of the silicon mass fraction in the liquid does not have the same issue with the liquid failing to reach the eutectic composition.

To examine the evolution in $C_{Si,liq}$ predicted using the UDF, the results are compared for the two methods and for the Scheil Equation at Point 3 and are shown in Figure 4.11. Point 3 is in a spoke and hub junction area where silicon composition in the liquid failed to reach the eutectic composition after solidification. The red line represents the silicon mass fraction calculated by the default FLUENT-based methodology and blue line by the UDS method. As can be seen, the composition of the liquid reaches 0.126 at $f_s$ of 0.68 for the UDS based method. The corresponding $f_{eut}$ would be 0.32, consistent with areas deplete due to bulk transport. It would appear that the default FLUENT-based methodology, under certain circumstances, yields a liquid composition below the eutectic at the point where solidification is completed, despite having input the eutectic composition of 0.126. In contrast, the results for the UDS method show that the eutectic composition is achieved in the liquid prior to completing solidification, consistent with what should be occurring. Thus, it would appear that the formulation adopted for the UDF address a shortcoming in FLUENT.
Taking a look at the overall mass fraction silicon, Figure 4.12 shows the contour calculated by FLUENT (RHS image) at 30s, which is close to the end of solidification (see white line $f_s = 1$, near the top of the hub). The results show that there is a band of material approximately mid-way in from the sides of the rim that appears slightly depleted in silicon. At the rim-spoke junction there are areas both depleted and enriched in silicon adjacent to each other and finally, a region depleted in silicon near the spoke/hub junction. Note: the red dot near the spoke/hub junction that appears in a region depleted in silicon. This is likely a numerical error and is investigated later in the sensitivity analysis.
Figure 4.12 Mass fraction of silicon in solid obtained through the UDS method (Left) and calculated by FLUENT (Right) at 30s

To take a more quantitative look at the silicon macrosegregation, the silicon profile has been plotted down the centreline of the rim and along the centre of the spoke in Figure 4.13 and Figure 4.14, respectively – see black lines in Figure 4.12 (RHS) for profile locations. As can be seen from these plots, the rim is generally enriched in silicon ($C_{Si,sol} > 0.07$) and the spoke is generally depleted ($C_{Si,sol} < 0.07$), apart from in proximity to the rim/spoke junction where the trend is opposite. Note: the large peak in the spoke associated with the red dot, which again appears to be a numerical error. Mechanistically, as liquid is drawn upward into the rim to feed the volumetric shrinkage associated with solidification, it becomes enriched in silicon as a result of micro-scale segregation associated with some solidification inward from the walls of the rim/spoke. Thus, the rim is generally enriched along its centreline and the spoke depleted. Relatively large variations in composition are predicted at the rim/spoke junction and near the hub, which appear to be related to the area of potential liquid encapsulation that forms at the rim/spoke junction.
To make a more quantitative comparison between the UDF and FLUENT-based results, the results for the UDF calculation were added to Figure 4.13 and Figure 4.14. The blue line represents the UDS for silicon mass fraction obtained via the UDF and the red line, the default method in FLUENT. Comparing the two, the results show the same qualitative trend and are in quantitative agreement to within less than 0.0012 mass fraction (0.12 wt.%) for the entire rim and most of the spoke, with the largest difference less than 0.0014 (0.14 wt.%) approximately at the rim/spoke junction. The reason for the differences observed between the two methods is not clear, as the FLUENT theory manual lacks sufficient detail to draw a conclusion. In the end, it was decided to proceed with the formulation of the UDF for hydrogen under the assumption that the difference was relatively small and likely within the ability to measure/predict other aspects of the industrial casting process – e.g. heat transfer, hydrogen-based porosity etc.

![Figure 4.13 Comparison of silicon mass fraction in solid profiles along rim centre](image-url)
4.5 Sensitivity Analysis

To explore the dependence of the model predictions on cooling rate, velocity attenuation in the mushy region, body force (gravity), mesh density and time-step, a sensitivity analysis was conducted by varying the relevant parameter in the model.

4.5.1 The Effect of Cooling Conditions

From the Equation 4.14, it can be seen that solute behaviour is determined by the liquid flow rate (advective term) and rate of change of \( f_i \) (source term). Both terms are strongly influenced by the cooling conditions, which are determined by the boundary conditions. Note: as a reminder, diffusive transport of solute has been ignored in the current analysis.

For the purpose of investigating the effect of cooling conditions on silicon macrosegregation, three cases with different thermal boundary conditions were explored. For the
sensitivity analysis, the numerical model described in section 4.4 was selected as the Reference Case. The boundary conditions used for the two other cases examined are shown in Table 4.2.

### Table 4.2 Boundary conditions used in the numerical models

<table>
<thead>
<tr>
<th>Reference case</th>
<th>Case 1</th>
<th>Case 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Encapsulation in spoke)</td>
<td>(directional solidification)</td>
<td>(Larger macrosegregation at rim/spoke joint)</td>
</tr>
<tr>
<td>@Top Adiabatic</td>
<td>@Top HTC = 500 (W/m²K)</td>
<td>@Top Adiabatic</td>
</tr>
<tr>
<td>@ Rim edges HTC = 2000 (W/m²K)</td>
<td>@ Rim edges HTC = 50 (W/m²K)</td>
<td>@ Rim edges HTC = 500 (W/m²K)</td>
</tr>
<tr>
<td>@ Spoke edges HTC = 1500 (W/m²K)</td>
<td>@ Spoke edges HTC = 50 (W/m²K)</td>
<td>@ Spoke edges HTC = 1500 (W/m²K)</td>
</tr>
</tbody>
</table>

The boundary conditions applied for Case 1 results in a significantly longer solidification time and a higher degree of directional solidification down the rim and across the spoke. Case 2 was chosen to create bi-directional solidification starting mid-spoke. Temperature contours for three cases at different times are shown in Figure 4.15 together with the black, grey and white contour lines. The loops formed by the grey line at 250s for Case 1 indicates that a region of semi-solid material is encapsulated at the spoke and hub transition. In Case 2, the solidification is completed first in the middle of the spoke, and then proceeds both toward the rim / spoke junction (and then up the rim) and toward the wheel hub. This cooling strategy would lead to the entire rim essentially encapsulated or cut off from feed liquid to offset solidification shrinkage.
Figure 4.15 Solidification sequence among three cases

Figure 4.16 shows comparisons of contours of the final solid mass fraction of silicon among three cases, near the end of solidification together with the superimposed black, grey and white iso-solid fraction lines. The predicted mass fraction of silicon in Case 2 shows a sharp increase in silicon at the rim/spoke junction and an area deplete in silicon at the spoke/hub junction, consistent with enriched liquid being drawn into the rim/spoke junction from the spoke/hub junction as it
flows through the inlet into the domain located at the top of the hub. The rim appears to solidify from bottom to top with very little segregation. As can be seen, the iso-solid fraction normal to the rim sides show only a slight degree of curvature and hence the solidification is largely unidirectional. This would tend to result in limited macrosegregation as the compensatory flow is parallel to the growth direction. Some flow normal to the solidification direction is necessary to transport the enriched liquid out from the grain envelope.

In Case 1, in contrast, there is a slight increase in the mass fraction of silicon found at the spoke/hub transition accompanied by a depletion zone. This develops in an area where the solidification pattern is complicated. Overall, the results clearly indicated that the cooling conditions have a significant effect on the solidification path, which in turn also significantly effects solute macrosegregation. Another interesting aspect of this result relates to how FLUENT accounts for areas of encapsulation that are cutoff from a source of liquid to feed solidification. In Case 2 the entire rim is cut-off and encapsulated. This would result in shrinkage porosity in an actual casting. It is unclear exactly how FLUENT deals with this in the context of the continuity equation, the increasing resistance to flow in the mushy zone and the evolution of pressure.

Figure 4.16 Silicon mass fraction predicted by three cases near the end of solidification
4.5.2 The Effect of Velocity Attenuation

In FLUENT, the mushy zone is treated as a porous medium, in which the resistance to liquid flow increases as $f_s$ increases. This resistance is accounted for via the addition of a momentum source term, shown expressed in Equation 4.5. In Equation 4.5, the parameter, $A_{mush} (kg/m^3.s)$, determines the extent or severity of velocity damping. As previously described in Section 4.1.2, the variable, $A_{mush} (kg/m^3.s)$, can be estimated via the liquid viscosity and the secondary dendrite arm spacing (SDAS). For the purpose of investigating the effect of velocity attenuation on the species macrosegregation and the evolution of pressure at locations of interest, $A_{mush} (kg/m^3.s)$ has been varied from $10^5$ (used in original reference or base-case model) to $10^8$ in increments of 10. Please note that $10^8$ corresponds to an average SDAS of 50 $\mu m$, which is near to typical values seen in an as-cast wheel. The results for silicon mass fraction applying different $A_{mush} (kg/m^3.s)$ values are shown in Figure 4.17.

![Figure 4.17](image)

(a) (b)
Figure 4.17 Silicon mass fraction predicted after solidification with different levels of attenuation in the mushy zone: (a) $A_{mush} = 10^5$, (b) $A_{mush} = 10^6$, (c) $A_{mush} = 10^7$ and (d) $A_{mush} = 10^8$.

The results show an almost identical distribution of silicon in the rim/spoke regions, where silicon is highly enriched at the rim/spoke junction and highly depleted in the vicinity of spoke/rim transition. Note: that the presence of the red dot in the area depleted in solute near the spoke/hub junction disappears as $A_{mush} (kg/m^3s)$ is increased from $10^5$ (used in original reference or base-case model) to $10^6$ confirming that its presence is likely a numerical instability or error.

To examine the effect of increasing $A_{mush} (kg/m^3s)$ more quantitative, profiles of the final Si mass fraction have been plotted along the centre of the line of the rim/spoke and are presented in Figure 4.18 and Figure 4.19 respectively, for the range of $A_{mush} (kg/m^3s)$ values examined. As can be seen, there appears to be little sensitivity to $A_{mush} (kg/m^3s)$ other than in the area of the spoke/hub junction that is depleted in the solute. Clearly, increasing $A_{mush} (kg/m^3s)$ from $10^5$ to $10^6$ has eliminated the peak at 0.037$m$, as previously discussed. It would also appear that this area is prone to instability in general.
Figure 4.18 Silicon mass fraction with different $Amush$ values along rim centre

Figure 4.19 Silicon mass fraction with different $Amush$ values along spoke centre
To further investigate the effect of $A_{mush} \text{(kg/m}^3\text{s)}$ on the evolution of the magnitude of velocity has been output from the model at three locations (see Figure 4.7 for locations) in Figure 4.20 through Figure 4.22. As a reminder, Point 1 corresponds to the location at the top rim where silicon is slightly enriched, Point 2 corresponds to the area in the rim/spoke junction that is significantly enriched and Point 3 corresponds to the location at spoke to hub transition where silicon is depleted. To provide a detailed view of velocity evolution at point 2, a zoomed in image is added to Figure 4.22. As can be seen from Figure 4.20 and Figure 4.21, the velocity gradually decreases at Points 1 and 3 as the liquid fraction is reduced. The behaviour at Point 2 is quite different and shows a peak in the range of $f_i = 0.5$ consistent with the eutectic reaction, which represents a sharp increase in the rate of solid fraction evolution with temperature. At all three locations, the results show that the peak velocity is decreased with increasing $A_{mush}(\text{kg/m}^3\text{s})$, which is counterintuitive, as increasing this term supports an increase in the attenuation of flow. One plausible explanation is that the increase in velocity magnitude is due to an increase in the degree of channelling that occurs. Referring back to Figure 4.4, the significant flow channel is observed at 5.5 and 8.5s. An increase in $A_{mush}(\text{kg/m}^3\text{s})$ would reduce the flow in areas of higher $f_s$ resulting in an increase in the flow at the centre line, consistent with what is observed. The large peak observed at Point 2 is consistent with the solidification of an area of increased silicon concentration and increased volume fraction of eutectic, which would cause a tremendous demand for the compensatory liquid to flow into the area as it undergoes the eutectic transformation.
Figure 4.20 Variation of velocity with fraction liquid for different $A_mush$ at Point 1

Figure 4.21 Variation of velocity with fraction liquid for different $A_mush$ at Point 3
Figure 4.22 Variation of velocity with fraction liquid for different $A_{mush}$ at Point 2: (a) in full velocity (b) expanded view up to $5 \times 10^{-3} \text{m/s}$
Another parameter of importance is pressure as the gradient in pressure drives flow and pressure is one of the critical parameters to predict porosity size distribution in the porosity model. Figure 4.23 shows a variation of pressure with fraction liquid for different $A_{mush} (kg/m^3 \cdot s)$ at Point 2. The output (gauge) pressure from FLUENT is measured relative to atmospheric pressure (101325 Pa).

![Figure 4.23 Variation of pressure with fraction liquid for different $A_{mush}$ at point 2](image)

As shown in Figure 4.23, the pressure drop induced by solidification shrinkage increases as solidification proceeds. As $A_{mush} (kg/m^3 \cdot s)$ increases from $10^5$ to $10^8$, the pressure drop is significantly increased from -350 Pa to -30000 Pa after solidification. For $A_{mush}$ values in the range of $10^7 – 10^8$, there is a significant increase in the rate of pressure drop associated with the eutectic transformation. $A_{mush} (kg/m^3 \cdot s)$ can be estimated from the SDAS size found in the actual as-cast wheel samples. As shown in Figure 4.24, the SDAS size in the rim/spoke junction area is in the range of 30 to 60 $\mu m$, which corresponds to $A_{mush} (kg/m^3 \cdot s)$ around $10^8$. Thus, the value of $10^8$ is
recommended to be assigned during the development of 3-D LPDC wheel casting model. However, a large input value of $A_{mush} (kg/m^3.s)$ requires a smaller time-step size to avoid numerical convergence issues, resulting in a significant increase in the simulation time.

Figure 4.24 Micrographs of a commercial production of A356 wheel at rim/spoke junction

4.5.3 The Effect of Body Force

As previously described, buoyancy driven flow has been ignored in the FLUENT-based model. The reference case in section 4.5.1 was used to test the effect of buoyancy (applied as a gravitational body force) on species macrosegregation in the domain and the evolution of pressure at Point 2. $A_{mush} (kg/m^3.s)$ was set to $10^8$ based on the previous analysis. The comparison of the predicted silicon distribution pattern is shown in Figure 4.25 and the direction of gravity is downward toward the rim/spoke joint, as labelled beside the contour on the right. The predict silicon mass fraction patterns are almost identical when the body force is included in the momentum conservation equation. A more quantitative look at of silicon mass fraction variation down the rim centreline and along spoke centreline, as shown in Figure 4.26 and Figure 4.27, indicates that the body force term has a negligible effect on the species macrosegregation. The evolution of pressure with fraction liquid is shown in Figure 4.28 and as can be seen the results are almost identical, matching the results for species macrosegregation. Thus, it can be concluded
that both species segregation and pressure evolution are insensitive to the body force term, in the 2-D simplified model.

Figure 4.25 Comparison of silicon mass fraction at 20s without gravity (Left) and with gravity (Right)

Figure 4.26 Comparison of silicon mass fraction along rim centre
Figure 4.27 Comparison of silicon mass fraction along spoke centre

Figure 4.28 Comparison of pressure variation with fraction liquid at Point 2
4.5.4 The Effect of Mesh Size

The sensitivity of silicon macrosegregation in the domain and evolution of pressure at Point 2 to the mesh size have been investigated. Once again, the reference case in Section 4.5.1 is applied to conduct the sensitivity analysis with the exception that $A_{mush} (kg/m^3.s)$ was set to $10^7$ instead of $10^5$ ($10^8$ was not used in order to reduce the calculation time and maintain model stability). The mesh is uniform with the size of 1mm in the FLUENT model. In order to test the effect of mesh size on species macrosegregation and the evolution of pressure at locations of interest, the mesh size was first increased to 2.5 mm then gradually reduced to 1.5mm, 1mm and 0.75mm. For reference, this corresponds to the number of volume element varying from 5 to 18 across the rim thickness.

The predicted silicon distribution patterns are shown in Figure 4.29. The superimposed black, grey and white $f_s$ contour lines have been included. In all cases, a similar silicon distribution pattern is yielded. As can be seen, the silicon macrosegregation does not change substantially when the mesh size is reduced below 1.5mm. Additionally, the calculation time was doubled as mesh size decreases from 1mm to 0.75mm. Given the increased calculation time and that the smallest mesh size (0.75mm) also shows what appears to numerical instability in the depletion zone in the spoke, the small mesh size was not adopted for further analysis. The evolution of pressure with fraction liquid at Point 2 is shown in Figure 4.30. Overall, the results show a similar trend, however, the pressure drop near the end of solidification ($f_l < 0.1$) predicted by the case adopting the smallest mesh size (0.75mm) is around 500Pa less than the other cases. In summary, an average mesh size of 1-1.5mm is recommended to predict species macrosegregation and describe the pressure drop at locations of interest.
Figure 4.29 Silicon mass fraction predicted by FLUENT model at 20s adopting different mesh sizes: a = 2.5mm, b = 1.5mm, c = 1mm, d = 0.75mm
4.5.5 The Effect of Time Step Size

A sensitivity to time step size was performed on the reference case model to test the effect on silicon macrosegregation and the evolution of pressure at Point 2. Based on the preceding analyses, the reference model was altered from its original formulation and adopted the mesh size of 1.5mm as well as $A_{mush} \text{ (kg/m}^3\text{s)}$ of $10^7$ in order to reduce computational time while maintaining stability. In the case of an axisymmetric formulation, only a constant time step size is allowed for the entire calculation. The maximum velocity (when $A_{mush} \text{ (kg/m}^3\text{s)} = 10^7$) reported in Figure 4.22 is 0.05 m/s. The base time step size was 0.002s, which was one magnitude lower than the ratio of the mesh size to the maximum velocity, which was 0.03. For the purpose of sensitivity analysis, the base time step size was further decreased to 0.0005s and then increased to 0.01 and 0.05s. The predicted silicon distribution patterns are shown in Figure 4.31 along with the $f_i$ contour lines. An
identical silicon distribution pattern is yielded. For the current FLUENT model, smaller time step size does not improve the accuracy of the silicon macrosegregation.

Figure 4.31 Silicon mass fraction predicted by the model at 20s with different time step sizes: a = 0.0005s, b = 0.002s, c = 0.01s, d = 0.05s

The evolution of pressure with fraction liquid at Point 2 is shown in Figure 4.32. Matching the trend above, decreasing time step size shows the negligible impact on the evolution of pressure at point 2. In summary, for the current FLUENT model, time step size 0.05s is small enough to provide stable results and offers the best balance between accuracy and computational cost.
4.6 Updates to the Hydrogen-Based Pore Model

*Hydrogen Macrosegregation* – In the original approach[46], the hydrogen concentration in the liquid, $C_{H,liq}$, was calculated based on the Scheil approximation taking into account the hydrogen reporting to pores (when present). To account for the potential for hydrogen segregation to affect porosity, the porosity model has been updated to utilize the $C_{H,liq}$ calculated from the UDF in FLUENT up to the eutectic transformation. In FLUENT, once the liquid mass fraction of silicon reaches the eutectic mass fraction of silicon at given points, the species conservation equations are no longer solved. Thus, both the liquid mass fractions of silicon and hydrogen are no longer updated for the balance of the solidification process. This makes sense for Si as the growth of the eutectic will not result in further local liquid enrichment. This is not the case for hydrogen. To address this and allow hydrogen partitioning throughout the entire solidification process, $C_{H,liq}$ is
input to the pore model from the FLUENT output file until the eutectic transformation occurs and then computed by mass conservation of hydrogen in the liquid\cite{46} via Equation 4.27:

\[ \Delta f_s \cdot C_{H,liq} \cdot (1-k_H) \cdot V_{vol} = \Delta \left( f_l \cdot C_{H,liq} \cdot V_{vol} \right) + \Delta \sum_i \left( \frac{N_{nucl} \cdot P \cdot V_g}{RT} \right)_i \]  

Equation 4.27

where \( V_{vol} (m^3) \) is the volume of the computational cell in FLUENT and \( k_H \) is the partition coefficient of hydrogen, \( T(K) \) is the temperature and \( R (J/mol/K) \) is the ideal gas constant. The left-hand-side of Equation 4.27 represents the amount of hydrogen rejected from the solid due to an increment in solid fraction, \( f_s \), as estimated based on the Scheil Equation, and the right-hand-side of Equation 4.27, represents the increase in hydrogen concentration in the liquid and the increase in the amount of hydrogen in the pores. The transition in updating \( C_{H,liq} \) from the value output from FLUENT to the Scheil approximation (See Equation 4.27) at a given point in the computational domain is dependent on the \( f_s \) at which the eutectic transformation occurs (\( f_{eut} \) - e.g. \( C_{Si,liq} = 0.126 \)) \( C_{H,liq} \) is based on the output data from FLUENT when \( f_s \) is less than \( f_{eut} \) and the Scheil Equation when \( f_s \) is greater than the \( f_{eut} \).

As can be seen in Figure 4.7, the eutectic transformation does not necessarily occur at an \( f_s \) of 0.5. Instead, it depends on macrosegregation and the \( f_s \) at which \( C_{Si,liq} = 0.126 \) is achieved. Therefore, the transition point is determined beforehand at each location by determining the \( f_s \) at which the liquid mass fraction of silicon reaches 0.126. Recall that the liquid mass fraction of silicon solved by the default methodology in FLUENT, under certain circumstances, falls short of the input eutectic composition of 0.126 (refer to Figure 4.11). To address this shortcoming, the liquid mass fraction of silicon obtained through the UDS method is used to determine the \( f_s \) at each location.
Pressure Evolution – The original model[46], did not account for the drop in pressure, $\Delta P_d (Pa)$, that can form at high solid fractions due to a decrease in permeability and therefore the effects of this pressure drop on pore nucleation and pore growth were ignored. The presence of a pressure drop can not only reduce the equilibrium saturation hydrogen concentration in the liquid, $C_i^e$ (see Equation 4.21), but also reduce the hydrogen concentration at liquid/pore interface $C_{lp}$ (see Equation 4.23). As a result, in the presence of a pressure drop, pores tend to form earlier due to a decrease in solubility limit and grow bigger due to a pressure-based increase in the hydrogen flux (see Equation 4.22). To account for this, the porosity model has been updated to utilize the local pressure output from FLUENT in the calculation of both the pore nucleation rate and pore growth rate expressions.

Shrinkage-based Pore Growth – As previously discussed, the maximum pressure drop was shown to be highly dependent on the velocity attenuation parameter ($A_{mush} (kg/m^3.s)$) in FLUENT. Due to the numerical convergence issues and excessively long execution times associated with high values of $A_{mush} (kg/m^3.s)$ the maximum value had to be restricted. As a result, it is likely that FLUENT will underestimate the magnitude of pressure drop experienced due to flow attenuation toward the end of mass feeding and more importantly in areas of liquid encapsulation at high $f_s$.

Given this limitation and the fact that some of the pores observed in actual castings are often small and tortuous in appearance, indicating they likely formed at a late stage in the solidification process, the porosity model has been revised to introduce a mechanism of pore growth based on conservation of volume in small areas of liquid encapsulation. In this approach, once late-stage liquid encapsulation/isolation occurs, the mass conservation (continuity) equation is modified such that solidification shrinkage is compensated only by the formation of porosity in
the liquid phase (assuming solid deformation can be ignored). Thus, the original mass conservation equation (see equation 4.2) is replaced with the following expression:

\[
\frac{\partial \rho}{\partial t} = \rho_l \frac{\partial f_p}{\partial t}
\]

Equation 4.28

where \(\rho\) (kg/m\(^3\)) is the overall density, \(\rho_l\) is the liquid density and \(f_p\) is the volume fraction of porosity. Setting the overall density to \(\rho = \rho_l f_l + \rho_s f_s\), the LHS of Equation 4.28 can be rewritten as \((\rho_s - \rho_l) \frac{\partial f_p}{\partial t}\), where \(\rho_s\) and \(\rho_l\) (kg/m\(^3\)) are constant and represent the solid and liquid densities, respectively. Equation 4.28 indicates the change in density (LHS) is solely compensated by pore growth (RHS). The change in pore volume fraction in the porosity model with time can then be computed via the following equation:

\[
\frac{\partial f_p}{\partial t} = \sum_{j=0}^{n_j} n_j \left[ \left( \frac{4\pi}{3} r_{pj}^3 \right)^{\nu+\Delta} \left( \frac{4\pi}{3} r_{pj}^3 \right)^{\nu} \right] / V \varphi
\]

Equation 4.29

where \(j\) and \(n_j\), respectively, represents the bin number and total number of pores in \(j_{th}\) bin and \(r_p\) (m) is the radius of growing pores associated with bin \(j\). Note: the pores nucleated within the same supersaturation range are binned and treated as a group in order to improve model efficiency[46]. The product of \(V \varphi\) represents the effective volume that pores can grow into. The impingement factor \(\varphi\) takes the identical form as Equation 4.22 to denote the resistance to pore growth from the growing dendritic structure.

The pore growth is related to the evolution of solid fraction by the following expression:

\[
V \varphi \frac{\rho_s - \rho_l}{\rho_l} \frac{\partial f_s}{\partial t} = \sum_{j=0}^{n_j} n_j \left[ \left( \frac{4\pi}{3} r_{pj}^3 \right)^{\nu+\Delta} \left( \frac{4\pi}{3} r_{pj}^3 \right)^{\nu} \right]
\]

Equation 4.30
Thus, pore growth at solid fractions in excess of the critical solid fraction for mass feeding is only controlled by the rate of solidification.

Implementation - The programming language Python 2.7 was used to update the original stand-alone porosity code to include the following modifications: 1) to input the evolution in liquid mass fraction of hydrogen computed by FLUENT using the UDF and to switch to a Scheil-based evolution at the $f_i$ consistent with the beginning of the eutectic reaction; 2) to input the evolution in pressure from FLUENT; and 3) to switch from a mass transfer-based pore growth mechanism to a shrinkage-based pore growth mechanism at a user-specified critical $f_s$.

Finally, FLUENT lacks the capability to accurately solve for the pressure evolution in large areas of liquid encapsulation that can arise in complex castings due to poor design and/or a poor choice of process parameters. This stems from the fact that the code maintains mass continuity throughout the domain. As a result, the pressure drop in areas that experience large volumes of liquid encapsulation will be not be accounted for. Pore formation in these areas is beyond the scope of the current project.

4.7 Microporosity Prediction in L-shaped Casting

As described in Chapter 3, the last stage of the work in this project was to predict the porosity size distribution at locations of interest in a production automotive wheel. The porosity model[46] is sequentially coupled with the FLUENT model. The input to the porosity model is composed of the evolution of pressure, temperature, fraction liquid and hydrogen concentration in the liquid, which are calculated within the FLUENT model. The evolution of hydrogen mass fraction in the liquid is computed via the UDF. The initial hydrogen mass fraction is $1.5 \times 10^{-7}$ (0.15ppm), which is slightly lower than the initial hydrogen content (0.2ppm) used in the reference[46] and is consistent with a 1-minute degassing treatment applied to a 0.6kg sample.
Note: that the FLUENT model is identical to the model developed in section 4.4. However, the $A_{mush} \text{ (kg/m}^3\text{s)}$ was set to $10^8$, to maximize the pressure drop toward the end of the mass feeding. The critical $f_s$ for shrinkage-based pore growth was set to 0.9 in the updated porosity model.

As previously described, the porosity model is used to predict the porosity size distribution at specific locations. The adjustable parameters $A$, $ss_0$ and $\sigma$ in the Gaussian nucleation function were set to those used for the 1.0 min degassed case in the reference[46]. $A$ represents the total number of available nucleation sites, which are determined by the total number of entrained oxides. $ss_0$ is the average hydrogen supersaturation required for pore nucleation. $\sigma$ represents the variability in the potency of nucleation sites, such as the geometry or composition of the solid substrates. The Gaussian nucleation function in the current study takes the following form:

$$
\frac{dN_{nuc}}{dss} = \frac{1.5}{\sqrt{2\pi \cdot 0.7}} \exp \left( -\frac{(ss - 1.7)^2}{2 \cdot 0.7^2} \right)
$$

Equation 4.31

Figure 4.33 shows the nucleation site distribution as a function of hydrogen supersaturation ($ss$). The peak of the curve corresponds to the average hydrogen supersaturation ($ss_0 = 1.7mol/m^3$) required for pore nucleation. The peak incremental increase in the number of pores within an increment in supersaturation occurs at $1.7mol/m^3$, whereas the nucleation process virtually ends when the local supersaturation exceeds $4mol/m^3$, having exhausted all of the heterogeneous nucleation sites.
4.8 Sensitivity Analysis on the Updated Porosity Model

4.8.1 The Effect of Hydrogen Concentration in Liquid ($C_{H,liq}$)

The $C_{H,liq}$ and its evolution with $f_s$ is one of the key factors in determining the pore size distribution. To explore the difference with respect to the evolution in $C_{H,liq}$ between the original porosity model and the updated version, the evolution in $C_{H,liq}$ at a location in the L-shape casting has been plotted as a function of $f_s$. The location chosen was near the “rim/spoke” junction in the L-shape casting – see Figure 4.7, Point 2 – which exhibits some enrichment. Figure 4.34 shows the results for both the Scheil-based approach (original[46]) and for the FLUENT-UDF-Scheil approach (updated) over the entire range in $f_s$ (a) and up to $f_s = 0.6$ (b). The corresponding hydrogen solubility, or the equilibrium saturation hydrogen concentration in the liquid, as a function of $f_s$ is also added to Figure 4.34 – see the yellow line. The difference between $C_{H,liq}$ and $C_{H,liq,\text{equilibrium}}$ represents the local supersaturation with respect to $f_s$. The red dash line indicates the $f_{\text{eu}}$ and its
corresponding hydrogen concentration in the liquid (~ 0.7mol/m$^3$). Note: in the updated approach, the amount of hydrogen in the gas phase when pores are present is not considered in the conservation equations solved in FLUENT. As shown in Figure 4.34, the $C_{H,liq}$ at Point 2 in the updated approach is higher than that obtained with the original approach by approximately 15-20% at an $f_s = 0.4$. However, as can be seen, on a percentage basis the increase becomes smaller with increasing $f_s$. The increase observed is consistent with macrosegregation predicted in FLUENT at this location indicating some net bulk transport of hydrogen into this area.

A comparison of the pore size distribution predicted by the different approaches (original[46] and updated) is shown in Figure 4.35, with the pore size distribution binned in 10-μm increments. The corresponding predicted porosity volume fraction by different approaches are shown in Figure 4.36. The updated approach predicts the formation of larger pores in the range of 90 to 100 μm (none were present in the original pore model), a fewer number are predicted in the bins representing 60-70 and 70-80 μm size range, and an increase is predicted in the bins representing 30-40, 40-50 and 50-60 μm. The expectation was an increase in the number density across the entire size range (consistent with a higher $C_{H,liq}$). The reason for this behaviour is not clear at this point in the sensitivity analysis.

The change in the overall volume fraction of porosity between the original and updated porosity models is plotted in Figure 4.36. As can be seen, the total porosity volume fraction is slightly increased relative to the original approach. Note: the effect of additional parameters on the volume fraction of porosity are added further into the sensitivity analysis.
Figure 4.34 Comparison of variation of $C_{H,\text{liq}}$ with liquid fraction $f_s$ at point 2: (a) full range in $f_s$, (b) expanded view up to $f_s = 0.6$. 
Figure 4.35 Comparison of pore size distribution between different approaches

Figure 4.36 Predicted porosity volume fraction by different approaches
4.8.2 The Effect of Velocity Attenuation Parameter ($A_{mush}$)

As described above, the evolution of pressure in the mushy regime, which is dependent on the $A_{mush}$ (kg/m$^3$.s) in FLUENT, will also influence pore formation and growth. To explore this, the evolution of pressure has been altered by changing $A_{mush}$ (kg/m$^3$.s) (recall that a higher value of $A_{mush}$ (kg/m$^3$.s) will result in a more significant pressure drop as solidification proceeds, see Figure 4.23). Figure 4.37 shows the effect of $A_{mush}$ (kg/m$^3$.s) on porosity size distribution.

![Figure 4.37 Comparison of pore size distribution among different $A_{mush}$](image)

As can be seen, the pore size distribution is shifted to an increased number density of large pores as $A_{mush}$ (kg/m$^3$.s) is increased (pressure drop increased) for a given initial melt hydrogen content and cooling conditions. By increasing the pressure drop, both the equilibrium value $C_e$ in Equation 4.21 and hydrogen concentration at the pore/liquid interface, $C_{lp}$, in Equation 4.23 will
decrease. As a result, pores nucleate at an earlier stage \((\text{supersaturation} = C_{\text{H,liq}} - C_f^*)\) and the mass transfer rate (see Equation 4.22) is increased due to an increase in the hydrogen concentration gradient, resulting in an increase in the number of large pore size and, based on hydrogen conservation, a reduction in the number of small pores. Figure 4.38 shows the predicted pore volume fraction as a function of \(A_{\text{mush}} \ (kg/m^3\cdot s)\). Increasing \(A_{\text{mush}} \ (kg/m^3\cdot s)\) from \(10^5\) to \(10^8\) results in an increase in porosity volume fraction from 0.12\% to 0.16\%.

![Figure 4.38 Comparison of porosity fraction among different \(A_{\text{mush}}\)](image)

4.8.3 The Effect of Critical \(f_s\)

As introduced above, the current model takes into account shrinkage based pore growth at high values of \(f_s\). Depending on as-cast morphology, the transition to shrinkage-based pore growth may take place at different solid fractions. Consequently, the sensitivity analysis was performed to investigate the effect of the critical solid fraction on prediction in pore size distribution (again Point 2 was used, see Figure 4.3). The base critical solid fraction for shrinkage growth was set to 0.9, identical to previous cases. The critical solid fraction was varied from 0.8 to 1.0 in increments.
of 0.05. With a value of 1.0 representing the case where the porosity model does not switch to a shrinkage-based evolution in porosity. All of the other model parameters were held constant.

The resulting predicted pore size distributions are shown in Figure 4.39. The shrinkage based pore growth mechanism shifts the number density to smaller pores, the opposite effect of increasing $A_{mush}$. Figure 4.40 shows the predicted porosity volume fraction as a function of the critical $f_s$ for shrinkage pore growth. The greater the critical $f_s$, the higher porosity volume fraction. Thus, switching to the shrinkage base pore growth model at an earlier stage impedes pore growth.

**Figure 4.39 Comparison of pore size distribution among different critical solid fractions**

The resulting predicted pore size distributions are shown in Figure 4.39. The shrinkage based pore growth mechanism shifts the number density to smaller pores, the opposite effect of increasing $A_{mush}$. Figure 4.40 shows the predicted porosity volume fraction as a function of the critical $f_s$ for shrinkage pore growth. The greater the critical $f_s$, the higher porosity volume fraction. Thus, switching to the shrinkage base pore growth model at an earlier stage impedes pore growth.
4.8.4 The Effect of Thermal Boundary Conditions

The sensitivity of the porosity model to the thermal boundary conditions was performed on three cases (see Table 4.2) to test the effect of boundary conditions on porosity prediction at Point 2 (see Figure 4.7). Note: that $10^7$ was assigned to the $A_{\text{mush}}$ (kg/m$^3$s) for three cases due to numerical instability when a greater $A_{\text{mush}}$ (kg/m$^3$s) is applied.

Recall that, relative to the Reference Case, the boundary conditions set for Case 1 were applied to achieve directional solidification, whereas for Case 2, mass feeding was cut off at an early stage of solidification and a relatively larger area of encapsulation was formed – see Section 4.5.1, Table 4.2. Also as a reminder, the evolution of hydrogen concentration in liquid, $f_s$ and pressure as a function of temperature are all inputs to the porosity model. Thus, to begin, the sensitivity of these parameters to the cooling conditions is presented first before examining the effect of cooling conditions on pore formation.
Figure 4.41 shows hydrogen mass fraction in liquid solved by the UDS method in FLUENT for different cases presented as a function of $f_s$ as input to the porosity model. *Note: the data plotted for each case is cut off at the point where the Eutectic composition is reached in the liquid and FLUENT no longer updates the conservation equations, which is around 0.5. At this point the porosity model switches to using the Scheil equation to estimate the evolution in $C_{H,liq}$."

In the plot, the blue line represents the variation of $C_{H,liq}$ with $f_s$ for the Base or Reference Case, the red for Case 1 and green line for Case 2. For the sake of comparison, the variation in $C_{H,liq}$ with $f_s$ calculated by Scheil equation has also been added and appears as the yellow dash line. As can be seen, the evolution in the hydrogen concentration in the liquid is sensitive to the cooling conditions. Case 1 conditions, representing directional solidification and the slowest cooling conditions, produced results virtually identical to Scheil behaviour. Whereas, both the Reference Case and Case 2 show hydrogen enrichment relative to Scheil behaviour at Point 2 indicating positive macro-segregation of hydrogen.

![Figure 4.41 Hydrogen mass fraction as a function of solid fraction among different cases](image_url)
The evolutions of temperature with respect to $f_s$ for different cases are shown in Figure 4.42. Likewise, the blue line represents the reference case while the green and red lines respectively for the Case 1 and Case 2. As can be seen, Case 1 clearly represent the slowest cooling rate relative to the Reference Case and Case 2. Furthermore, the amount of eutectic increases in the Reference Case and Cases 2 relative to Case 1, as indicated by the lower solid fraction when the “plateau” in temperature occurs associated with eutectic transformation at 577°C. This is consistent with Point 2 being enriched in Si due to macro-segregation in the Reference Case and Cases 2 (as well as hydrogen).

![Figure 4.42 Temperature as a function of solid fraction among different cases](image-url)
The last key factor in determining the pore size distribution is the local evolution of pressure, which has been plotted in Figure 4.43. To provide a more detailed view of the maximum pressure drop during solidification at Point 2 for the Reference Case and Case 1, the pressure range on the y-axis was limited to between 0 and -40000 Pa and is replotted in Figure 4.43. As before, the blue line represents the variation of pressure with $f_s$ for the reference case. The green and red lines represent the results for Cases 1 and 2, respectively.
Figure 4.43 Pressure drop as a function of solid fraction at point 2 among different cases: (a) full range in pressure, (b) expanded view up to -4000 Pa

As can be seen, the evolution in the pressure predicted by FLUENT is highly sensitive to the cooling conditions in the L-shape casting at Point 2, with the maximum pressure decrease ranging from around 350 Pa (Case 1) to $1.5 \times 10^5$ Pa (Case 2). Case 2, represents the cooling conditions that led to a significant volume of liquid encapsulation in the rim adjacent to Point 2. Hence the large pressure drop associated with the eutectic reaction as the material undergoing the transformation is cut-off from a supply of liquid. In fact, Case 2 was unable to run to completion as the solution failed to converge. Practically speaking, the maximum pressure drop should approximately coincide with either the vapour pressure of hydrogen or aluminum, in solution, whichever is higher. At Point 2 in the L-shape casting, the vapour pressure of hydrogen exceeds the local pressure at $f_s$ of approximately 0.5 for an initial hydrogen concentration of 0.15ppm (see Figure 4.44, the local pressure is denoted by the red line while the vapour pressure of hydrogen in
blue). Certainly, pressure drops in excess of 101325 Pa (1 atm) are not possible. The excessively large and erroneous pressure drop predicted by FLUENT is not unexpected as FLUENT assumes continuity throughout the domain – i.e. the mass continuity equation is not formulated to allow for the formation of a gas phase as would be expected to occur at Point 2, Case 2. To address this shortcoming, in the updated porosity model the minimum local pressure is limited to 60,000 Pa (see Figure 4.44), which is consistent with when hydrogen-based pore formation would occur in the system under consideration.

![Figure 4.44 Local pressure and the vapour pressure of hydrogen pore as a function of solid fraction at point 2, Case 2](image)

The effect of the pressure drop predicted in the Reference Case and in Case 2, are significant and would be expected to have an impact on pore nucleation and growth. The pressure drop predicted for the directional solidification conditions attained in Case 1, would not be expected to influence pore formation.
The corresponding model predictions in pore size distribution for different cases are shown in Figure 4.45, with the pore size distribution binned in 10-μm increments. The model prediction for the Reference Case is shown in blue, while the green and red bars represent the pore size distributions for Case 1 and Case 2, respectively. As expected, the maximum pore radius increases from 100 μm to 150 μm as pressure drop increases from -3000 Pa to -60000 Pa. (Reference Case vs. Case 2). Whereas the maximum pore radius decreases from 100 μm to 30 μm as pressure drop decreases from -3000 Pa to -300 Pa. It can be concluded that the pressure evolution exerts a substantial effect on pore size distribution in the current porosity model. Large pressure drops can promote pores to form earlier resulting in larger pores.

Figure 4.45 Comparison of pore size distribution among different cases
5 Low Pressure Die Casting Process

The thermal-flow-compositional model developed in the previous chapter is now used to examine the role of silicon macrosegregation on liquid encapsulation and the role of hydrogen macrosegregation, pressure evolution and cooling rate on pore formation in LPDC A356 automotive wheels. In this Chapter, a 3-D numerical model has been developed to simulate solidification in a wheel in a multicomponent alloy, Al-7wt.%Si-0.3wt.%Mg, (similar to A356). Section 5.1 focuses on the model development including the solution technique, the computational domain, the material properties, and the initial and boundary conditions. Following this, Section 5.2 compares the simulation results for temperature and Si-segregation against measured plant trial data and examines the effect of Si-segregation on the prediction of liquid encapsulation. Finally, Section 5.3 concentrates on the application of the porosity model to predict the pore size distribution at discrete locations in a commercially produced A356 wheel.

5.1 LPDC Model Development

The LPDC model was developed based on the thermal-fluid-composition model from Chapter 4 and it was applied to predict silicon and hydrogen macrosegregation during solidification of an LDPC wheel. An incremental approach is used to obtain the final solution. Initially, the model is repeatedly run in a thermal diffusion only mode until the die temperature reaches cyclic steady state – e.g. until the die temperature at the end of given cycle does not change significantly (<10°C) from cycle-to-cycle. Following this, the model is then run considering fluid flow and solute segregation in addition to temperature. This is done to limit the number of times the fully coupled model has to be run. The LPDC model was initially developed based on ABAQUS by Reilly et al. in the casting group at University of British Colombia. In the current
study, the above model was rebuilt in FLUENT 16.0 with updates so as to investigate species macrosegregation during solidification of an A356 wheel casting.

For simulation of the wheel casting, the residuals for the convergence criterion were set to $10^{-6}$ for energy, $10^{-3}$ for continuity and velocity and $10^{-5}$ for species. A fixed time step size of 0.5s was used in the thermal diffusion-only model, whereas an adaptive time stepping method was applied to the fully coupled model in order to ensure model stability. One cycle of the thermal-only model took approximately 16 $hrs.$ to run on 4 Intel(R) Xeon(R) CPUs (2.33GHz), whereas one cycle of the thermal-fluid-composition code would typically take more than 1000 $hrs.$

The fully coupled model incorporates the relevant solidification phenomena including mushy zone resistance (Darcy flow damping), latent heat evolution, and solute partitioning during the phase change. The effect of gravity on flow has been neglected – e.g. there is no thermal or solutal buoyancy. Thus, the driving force for flow is volume conservation associated with the density change during solidification. In addition, the solid phase is fixed. Thus the solid momentum equation is not considered.

**Computational Domain**

The model geometry was based on a five-spoke wheel. A 36° section of the die and wheel was adopted in order to reduce computational time. The geometry in the model is shown in Figure 5.1, which includes eleven components. The size and location of the cooling channels in the die have been hidden at the request of the collaborating company. The geometry was meshed in ANSYS Workbench and contained 1,954,807 tetrahedron elements in total. The face area of the mesh elements ranges from $5.15 \times 10^{-2} \, mm^2$ to 214 $mm^2$. Note: that the coarse mesh can lead to small gaps between mating components with high curvature. As a result, a refined mesh was assigned at the high curvature interfaces to avoid gap formation between matching components.
Figure 5.2 shows an example of the mesh adopted at the wheel and the die interfaces within the expanded region contained within the red circle shown in Figure 5.1.
**Material Properties**

The wheel material was A356 and approximated as Al-7wt.%Si-0.3wt.%Mg. All the die components were made of H13 tool steel, except for upper sprue, which was made of tungsten carbide. The thermophysical properties[13][60][17][62][63][64] for the wheel and die materials used in the model are given in Table 5.1. Note that the density of the solid and liquid phases was assumed to be constant. The density in the mushy zone was calculated according to Equation 5.1, where \( f_i \) is liquid fraction.

\[
\rho = \rho_l f_i + \rho_s (1 - f_i)
\]

Equation 5.1

A similar approach was adopted to calculate thermal conductivity.

<table>
<thead>
<tr>
<th>Material</th>
<th>Properties</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>A356</td>
<td>Thermal conductivity of Solid</td>
<td>70</td>
<td>W/m.K</td>
</tr>
<tr>
<td></td>
<td>Thermal conductivity of liquid</td>
<td>135</td>
<td>W/m.K</td>
</tr>
<tr>
<td></td>
<td>Specific heat, ( C_p )</td>
<td>1150</td>
<td>J/kg.K</td>
</tr>
<tr>
<td></td>
<td>Latent Heat, ( L )</td>
<td>397500</td>
<td>J/kg</td>
</tr>
<tr>
<td></td>
<td>Density of Solid, ( \rho_s )</td>
<td>2685</td>
<td>kg/m(^3)</td>
</tr>
<tr>
<td></td>
<td>Density of liquid, ( \rho_l )</td>
<td>2540</td>
<td>kg/m(^3)</td>
</tr>
<tr>
<td></td>
<td>Viscosity of the liquid, ( \mu_l )</td>
<td>0.0014</td>
<td>kg/m.s</td>
</tr>
<tr>
<td></td>
<td>Partition Coefficient of Si, ( k_{Si} )</td>
<td>0.13</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Partition Coefficient of Mg, ( k_{Mg} )</td>
<td>0.48</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Slope of the liquidus, ( m_{Si} )</td>
<td>658.73</td>
<td>K/wt%</td>
</tr>
<tr>
<td></td>
<td>Slope of the liquidus, ( m_{Mg} )</td>
<td>589.88</td>
<td>K/wt%</td>
</tr>
<tr>
<td></td>
<td>Si diffusion coefficient in liquid ( D_{Si,liq} )</td>
<td>Ignored</td>
<td>m(^2)/s</td>
</tr>
<tr>
<td></td>
<td>Mg diffusion coefficient in liquid ( D_{Mg,liq} )</td>
<td>Ignored</td>
<td>m(^2)/s</td>
</tr>
<tr>
<td></td>
<td>Si diffusion coefficient in solid ( D_{Si,sol} )</td>
<td>Ignored</td>
<td>m(^2)/s</td>
</tr>
<tr>
<td></td>
<td>Mg diffusion coefficient in solid ( D_{Mg,sol} )</td>
<td>Ignored</td>
<td>m(^2)/s</td>
</tr>
<tr>
<td>H13</td>
<td>Density ( \rho )</td>
<td>7800</td>
<td>kg/m(^3)</td>
</tr>
<tr>
<td></td>
<td>Specific heat, ( C_p )</td>
<td>460</td>
<td>J/kg.K</td>
</tr>
<tr>
<td></td>
<td>Thermal conductivity, ( \lambda )</td>
<td>24.4</td>
<td>W/m.K</td>
</tr>
<tr>
<td>Tungsten carbide</td>
<td>Density ( \rho )</td>
<td>1560</td>
<td>kg/m(^3)</td>
</tr>
<tr>
<td></td>
<td>Specific heat, ( C_p )</td>
<td>210</td>
<td>J/kg.K</td>
</tr>
<tr>
<td></td>
<td>Thermal conductivity, ( \lambda )</td>
<td>84.2</td>
<td>W/m.K</td>
</tr>
</tbody>
</table>
*The density of the solid and the liquid phases are dependent on temperature, however the model adopted a constant value for each phase for the sake of simplicity. A different density value for each phase will inevitably change the volume shrinkage ratio of A356. In turn, it will affect the fluid flow which is induced by the solidification shrinkage. Due to extremely long running time, the opportunity to investigate the potential effect of different density values on fluid flow was greatly undermined.

Initial conditions

As described above, an incremental approach is used to obtain the final casting process solution. Initially, the model was run in a thermal only model, starting from a uniform die temperature of 500°C and a uniform wheel temperature of 700°C. (Note: die cavity filling was not simulated). Following the initial run, the model was then run repetitively using the temperature distribution within the die at the end of the previous cycle as the initial condition for the die temperature in the current cycle. The initial wheel temperature remained 700°C for every cycle. The model was run in this manner until the temperature distribution within the various die components reached the cyclic steady state (after approximately 10 cycles) to within a user-specified tolerance. Once a cyclic steady state condition was approximately achieved, fluid flow and species transport were switched on. The initial mass fraction of silicon and magnesium in the fully coupled model were 7wt.% and 0.3wt.% respectively. The initial hydrogen mass fraction was assumed to be $1.5\times10^{-5}$wt.% (0.15ppm). Note: 1) Unfortunately, the initial mass fraction of hydrogen could not be easily measured in the industrial setting because of the continuous hydrogen degassing and two-chamber system that is used in the holding furnace at the industrial collaborators facility; and 2) the mass fraction of hydrogen was assumed to be 0.05ppm less than
the lowest hydrogen content in reference[46], reflecting continuous degassing that is used in the commercial process.

**Boundary conditions**

It takes approximately 180s to complete one cycle of the LPDC process, which was comprised of the following 4 steps, or stages, from the standpoint of how the basic boundary conditions change within a cycle:

*Process Step 1 (0-28s)* - Top die is moved down, side dies are closed and in contact with bottom die and the die cavity is filled;

*Based on thermocouple data, the wheel started to solidify at around the 28th second. The filling process was not simulated in the model.*

*Process Step 2 (28-117s)* – The wheel is solidified;

*Step 3 (117-132s)* - Side dies are opened and the contact is lost between the various die components. The top die is raised with the wheel attached due to thermal contraction;

*Step 4 (132-180s)* - Wheel was removed from the top die and all of the internal surfaces of the die were exposed to the environment.

Interfacial heat transfer between the wheel and die, the various die interfaces and between the various die component and the environment was included in each step and applied where/when appropriate based on the state of the process.

FLUENT applies a thermally coupled wall boundary to simulate interfacial heat transfer at interfaces. In this case, the liquid domain (the wheel) is not permitted to enter the solid domain (the die) and vice versa. The heat flux between coupled walls is given as:

\[ q = h(T_{w1} - T_{w2}) \]  

Equation 5.2
where \( h \, (W/m^2\cdot K) \) is the interfacial heat transfer coefficient and \( T_{W1} \, (K) \) and \( T_{W2} \, (K) \) are the surface temperatures of interface walls. The effect of gap formation between the wheel and the die on the interfacial heat transfer coefficient during solidification was taken into account by assigning a series of temperature dependent interfacial heat transfer coefficients, dependent on location. In all cases, the interfacial heat transfer coefficients are constant and high above the liquidus temperature and then linearly dropped to relatively low values at the eutectic temperature. Following this, the interfacial heat transfer coefficient remained unchanged for the balance of the solidification stage. Table 5.2 shows the interfacial heat transfer coefficients applied to the wheel/die interfaces. At the current stage of model development, the contact resistance between mating die components was ignored.

<table>
<thead>
<tr>
<th>Interface</th>
<th>Temperature (K)</th>
<th>Heat transfer coefficient (W/m²·K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bottom die/Wheel</td>
<td>( T \geq 884.15 )</td>
<td>2500 (strong contact)</td>
</tr>
<tr>
<td></td>
<td>( 884.15 &gt; T &gt; 845.15 )</td>
<td>( 2500 + 51.28 \times (T-884.15) )</td>
</tr>
<tr>
<td></td>
<td>( T \leq 845.15 )</td>
<td>500 (weak contact)</td>
</tr>
<tr>
<td>Centre pin/Wheel</td>
<td>( T \geq 884.15 )</td>
<td>2500</td>
</tr>
<tr>
<td></td>
<td>( 884.15 &gt; T &gt; 845.15 )</td>
<td>( 2500 + 51.28 \times (T-884.15) )</td>
</tr>
<tr>
<td></td>
<td>( T \leq 845.15 )</td>
<td>500</td>
</tr>
<tr>
<td>Side die/Wheel</td>
<td>( T \geq 884.15 )</td>
<td>1500</td>
</tr>
<tr>
<td></td>
<td>( 884.15 &gt; T &gt; 845.15 )</td>
<td>( 1500 + 25.64 \times (T-884.15) )</td>
</tr>
<tr>
<td></td>
<td>( T \leq 845.15 )</td>
<td>500</td>
</tr>
<tr>
<td>Side die drum core/Wheel</td>
<td>( T \geq 884.15 )</td>
<td>1500</td>
</tr>
<tr>
<td></td>
<td>( 884.15 &gt; T &gt; 845.15 )</td>
<td>( 1500 + 25.64 \times (T-884.15) )</td>
</tr>
<tr>
<td></td>
<td>( T \leq 845.15 )</td>
<td>500</td>
</tr>
<tr>
<td>Top die/Wheel</td>
<td>( T \geq 884.15 )</td>
<td>5500</td>
</tr>
<tr>
<td></td>
<td>( 884.15 &gt; T &gt; 845.15 )</td>
<td>( 5500 + 128.21 \times (T-884.15) )</td>
</tr>
<tr>
<td></td>
<td>( T \leq 845.15 )</td>
<td>500</td>
</tr>
<tr>
<td>Top die thermal break/Wheel</td>
<td>( T \geq 884.15 )</td>
<td>3500</td>
</tr>
<tr>
<td></td>
<td>( 884.15 &gt; T &gt; 845.15 )</td>
<td>( 3500 + 76.92 \times (T-884.15) )</td>
</tr>
<tr>
<td></td>
<td>( T \leq 845.15 )</td>
<td>500</td>
</tr>
<tr>
<td>Top die drum core/Wheel</td>
<td>( T \geq 884.15 )</td>
<td>2500</td>
</tr>
<tr>
<td></td>
<td>( 884.15 &gt; T &gt; 845.15 )</td>
<td>( 2500 + 51.28 \times (T-884.15) )</td>
</tr>
<tr>
<td></td>
<td>( T \leq 845.15 )</td>
<td>500</td>
</tr>
</tbody>
</table>
Upper sprue/Wheel

\[ T \geq 884.15 \]
\[ 884.15 > T > 845.15 \]
\[ T \leq 845.15 \]

3000
\[ 3000 + 64.1 \times (T - 884.15) \]

500

As mentioned above, heat transfer to the environment by radiation and convection occurred through the entire LPDC process. Table 5.3 shows the combined convection/radiation boundary condition applied in the model.

Table 5.3 Combined convection/radiation boundary condition

<table>
<thead>
<tr>
<th>Location</th>
<th>Step</th>
<th>HTC ((W/m^2 K))</th>
<th>External Temperature((K))</th>
<th>External Emissivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bottom die</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>External Surface</td>
<td>1-4</td>
<td>20</td>
<td>453.15</td>
<td>0.7</td>
</tr>
<tr>
<td>Frame</td>
<td>1-4</td>
<td>50</td>
<td>481.15</td>
<td></td>
</tr>
<tr>
<td>Mating surface with top die drum core</td>
<td>1</td>
<td>20</td>
<td>323.15</td>
<td>0.7</td>
</tr>
<tr>
<td></td>
<td>3-4</td>
<td>20</td>
<td>323.15</td>
<td>0.6</td>
</tr>
<tr>
<td>Contact surface with wheel</td>
<td>1</td>
<td>20</td>
<td>323.15</td>
<td>0.7</td>
</tr>
<tr>
<td></td>
<td>3-4</td>
<td>20</td>
<td>323.15</td>
<td>0.6</td>
</tr>
<tr>
<td>Mating surface with side die drum core</td>
<td>3-4</td>
<td>20</td>
<td>323.15</td>
<td>0.6</td>
</tr>
<tr>
<td>Centre pin</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>External surface</td>
<td>1-4</td>
<td>20</td>
<td>368.15</td>
<td>0.7</td>
</tr>
<tr>
<td>Centre pin tip</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Contact surface with wheel</td>
<td>1</td>
<td>20</td>
<td>323.15</td>
<td>0.7</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>20</td>
<td>323.15</td>
<td>0.6</td>
</tr>
<tr>
<td>Side die</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>External surface</td>
<td>1-4</td>
<td>35</td>
<td>403.15</td>
<td>0.7</td>
</tr>
<tr>
<td>Mating surface with top die thermal break</td>
<td>1</td>
<td>20</td>
<td>323.15</td>
<td>0.7</td>
</tr>
<tr>
<td></td>
<td>3-4</td>
<td>20</td>
<td>323.15</td>
<td>0.6</td>
</tr>
<tr>
<td>Surface faces side die drum core</td>
<td>1-4</td>
<td>20</td>
<td>608.15</td>
<td>0.7</td>
</tr>
<tr>
<td>Contact surface with wheel</td>
<td>1</td>
<td>20</td>
<td>323.15</td>
<td>0.7</td>
</tr>
<tr>
<td></td>
<td>3-4</td>
<td>20</td>
<td>323.15</td>
<td>0.6</td>
</tr>
<tr>
<td>Side die drum core</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Surface faces bottom die</td>
<td>1-4</td>
<td>50</td>
<td>423.15</td>
<td>0.7</td>
</tr>
<tr>
<td>--------------------------</td>
<td>-----</td>
<td>----</td>
<td>--------</td>
<td>-----</td>
</tr>
<tr>
<td>External surface</td>
<td>1-4</td>
<td>50</td>
<td>423.15</td>
<td>0.7</td>
</tr>
<tr>
<td>Surface faces side die</td>
<td>1-4</td>
<td>50</td>
<td>423.15</td>
<td>0.7</td>
</tr>
<tr>
<td>Contact surface with wheel</td>
<td>1</td>
<td>20</td>
<td>323.15</td>
<td>0.7</td>
</tr>
<tr>
<td></td>
<td>3-4</td>
<td>20</td>
<td>323.15</td>
<td>0.6</td>
</tr>
<tr>
<td>Mating surface with bottom die</td>
<td>3-4</td>
<td>20</td>
<td>323.15</td>
<td>0.6</td>
</tr>
</tbody>
</table>

**Top die**

<table>
<thead>
<tr>
<th>Surface faces top die drum core</th>
<th>1-4</th>
<th>20</th>
<th>368.15</th>
<th>0.7</th>
</tr>
</thead>
<tbody>
<tr>
<td>External surface</td>
<td>1-4</td>
<td>20</td>
<td>403.15</td>
<td>0.7</td>
</tr>
<tr>
<td>Frame</td>
<td>1-4</td>
<td>500</td>
<td>413.15</td>
<td></td>
</tr>
<tr>
<td>Contact surface with wheel</td>
<td>1</td>
<td>20</td>
<td>323.15</td>
<td>0.7</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>20</td>
<td>323.15</td>
<td>0.6</td>
</tr>
</tbody>
</table>

**Top die thermal break**

<table>
<thead>
<tr>
<th>External surface</th>
<th>1-4</th>
<th>20</th>
<th>403.15</th>
<th>0.7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mating surface with side die</td>
<td>1</td>
<td>20</td>
<td>323.15</td>
<td>0.7</td>
</tr>
<tr>
<td></td>
<td>3-4</td>
<td>20</td>
<td>323.15</td>
<td>0.6</td>
</tr>
<tr>
<td>Contact surface with wheel</td>
<td>1</td>
<td>20</td>
<td>323.15</td>
<td>0.7</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>20</td>
<td>323.15</td>
<td>0.6</td>
</tr>
</tbody>
</table>

**Top die drum core**

<table>
<thead>
<tr>
<th>External surface</th>
<th>1-4</th>
<th>20</th>
<th>368.15</th>
<th>0.7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Contact surface with wheel</td>
<td>1</td>
<td>20</td>
<td>323.15</td>
<td>0.7</td>
</tr>
<tr>
<td></td>
<td>4</td>
<td>20</td>
<td>323.15</td>
<td>0.6</td>
</tr>
</tbody>
</table>

**Upper sprue**

| Contact surface with wheel    | 1   | 20 | 323.15 | 0.7 |
|                              | 3-4 | 20 | 323.15 | 0.6 |

**Wheel**

| Contact surface with side die, bottom die, upper sprue, side die drum core | 3   | 20 | 323.15 | 0.6 |

There are six cooling channels in the die and water is used as the cooling media. The current model takes into account the change in heat transfer coefficient when the water changes from
stagnant to flowing in the cooling channels. *Note: the interfacial heat transfer coefficient used in the cooling channels does not consider water boiling, which may be occurring when water is first introduced into a channel that has become dry.* Table 5.4 shows the cooling channel boundary conditions applied in each cycle.

Table 5.4 Cooling channel boundary conditions

<table>
<thead>
<tr>
<th>Cooling Channel</th>
<th>HTC (W/m²K)</th>
<th>Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Bottom die 1</strong></td>
<td>100 (Stagnant)</td>
<td>time &lt; 78</td>
</tr>
<tr>
<td></td>
<td>100+(time-78)×6400/5</td>
<td>78 &lt;= time &lt; 83</td>
</tr>
<tr>
<td></td>
<td>6500 (Flowing)</td>
<td>83 &lt;= time &lt; 168</td>
</tr>
<tr>
<td></td>
<td>6500-(time-168)×6400/5</td>
<td>168 &lt;= time &lt; 173</td>
</tr>
<tr>
<td></td>
<td>100 (Stagnant)</td>
<td>173 &lt;= time &lt; 180</td>
</tr>
<tr>
<td><strong>Bottom die 2</strong></td>
<td>200 (Stagnant)</td>
<td>time &lt; 48</td>
</tr>
<tr>
<td></td>
<td>200+(time-48)×10800/10</td>
<td>48 &lt;= time &lt; 58</td>
</tr>
<tr>
<td></td>
<td>11000 (Flowing)</td>
<td>58 &lt;= time &lt; 78</td>
</tr>
<tr>
<td></td>
<td>11000-(time-78)×10800/10</td>
<td>78 &lt;= time &lt; 88</td>
</tr>
<tr>
<td></td>
<td>200 (Stagnant)</td>
<td>88 &lt;= time &lt; 180</td>
</tr>
<tr>
<td><strong>Centre pin</strong></td>
<td>5500 (Stagnant)</td>
<td>time &lt; 108</td>
</tr>
<tr>
<td></td>
<td>5500+(time-108)×1000/5</td>
<td>108 &lt;= time &lt; 103</td>
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<tr>
<td></td>
<td>6500 (Flowing)</td>
<td>103 &lt;= time &lt; 158</td>
</tr>
<tr>
<td></td>
<td>6500-(time-158)×1000/5</td>
<td>158 &lt;= time &lt; 163</td>
</tr>
<tr>
<td></td>
<td>5500 (Stagnant)</td>
<td>163 &lt;= time &lt; 180</td>
</tr>
<tr>
<td><strong>Side die drum core</strong></td>
<td>500 (Stagnant)</td>
<td>time &lt; 8</td>
</tr>
<tr>
<td></td>
<td>500+(time-8)×7000/5</td>
<td>8 &lt;= time &lt; 13</td>
</tr>
<tr>
<td></td>
<td>7500 (Flowing)</td>
<td>13 &lt;= time &lt; 180</td>
</tr>
<tr>
<td><strong>Top die drum core</strong></td>
<td>9000 (Stagnant)</td>
<td>time &lt; 68</td>
</tr>
<tr>
<td></td>
<td>9000+(time-68)×1000/10</td>
<td>68 &lt;= time &lt; 78</td>
</tr>
<tr>
<td></td>
<td>10000 (Flowing)</td>
<td>78 &lt;= time &lt; 158</td>
</tr>
<tr>
<td></td>
<td>10000-(time-158)×1000/10</td>
<td>158 &lt;= time &lt; 168</td>
</tr>
<tr>
<td></td>
<td>9000 (Stagnant)</td>
<td>168 &lt;= time &lt; 180</td>
</tr>
<tr>
<td><strong>Top die pond</strong></td>
<td>100 (Stagnant)</td>
<td>time &lt; 8</td>
</tr>
<tr>
<td></td>
<td>100+(time-8)×1650/5</td>
<td>8 &lt;= time &lt; 13</td>
</tr>
<tr>
<td></td>
<td>1750 (Flowing)</td>
<td>13 &lt;= time &lt; 180</td>
</tr>
</tbody>
</table>

* The parameters provided in Table 5.2 through Table 5.4 were based on the studies conducted by Dr. Carl Reilly in the casting group at University of British Colombia and on previously
published work[62]. He adopted the trial-and-error method to arrive at a set of HTC values that gave the “best fit” to the thermocouple data for both the wheel and the die.

In order to compensate for the volume change that occurs during solidification, the bottom surface of the wheel hub was defined as a pressure inlet boundary. Material introduced at this boundary enters with the same temperature and solute content as the material in the wheel directly adjacent to the boundary.

5.2 Result and Discussion

Thermocouple locations - Several thermocouples were placed at various locations on the external surfaces of the die sections during a plant trial. A couple of them as shown in Figure 5.3 were selected to provide basic validation of the evolution of temperature of the die components within a cycle.

Figure 5.3 Thermocouple locations on various die components
Additionally, several thermocouples were solidified into the wheel – see locations A through E in Figure 5.4 – to provide data to verify the evolution of temperature within the wheel within a cycle.

![Figure 5.4 Thermocouple locations within the wheel](image)

**Figure 5.4 Thermocouple locations within the wheel**

*Thermal Predictions and Comparison to Thermocouple Data* - The results comparing the model predictions with the measurements taken from the die are shown in Figure 5.5 through Figure 5.8 for the fully coupled thermal-fluid-composition simulation. The measured data are shown as dashed lines while the model predictions are shown as solid lines. As can be seen, the plot shows relatively good agreement between the two, except for location TC_3 on the side die. *Note: that the model in the current study did not include a heater located on the outside surface of the side die and is used in the current commercial process to add heat periodically when the temperature in the side die drops below a set-point temperature. Thus, the heat flows in the side die are not correctly characterized, which likely contributed to the discrepancy between model prediction and measured data observed at TC_3.*
Figure 5.5 Comparison between experimental data (dash) and simulated (solid) temperatures at top die
core

Figure 5.6 Comparison between experimental data (dash) and simulated (solid) temperatures at top die drum
core
Figure 5.7 Comparison between experimental data (dash) and simulated (solid) temperature at bottom die

Figure 5.8 Comparison between experimental data (dash) and simulated (solid) temperature at side die
Figure 5.9 Comparison between experimental data (dash) and simulated (solid) temperatures in the wheel at location A, B and C.

Figure 5.10 Comparison between experimental data (dash) and simulated (solid) temperatures in the wheel at location D and E.
Figure 5.9 and Figure 5.10 show comparisons between the measured and predicted temperature evolution at five locations in the wheel. The measured data are shown as dashed lines, while predictions from the fully coupled model are solid lines. *(Note: that the comparison is cut off when solidification in the wheel is complete).* Overall the results show good qualitative agreement in terms of the shape of the cooling curves and the trend at the different locations. The most significant error is observed at location A, which is at the top of the rim. At location A, the eutectic transformation is predicted to be completed at 22s, whereas the TC data indicates it is completed at approximately 36s. The top of the rim is known to have complex behaviour in terms of the evolution of the interface resistance, as there are areas where gap forms and areas that are under pressure – *e.g.* the interfaces are forced together. One possible explanation for the poor agreement in this area is that the evolution in HTC is not described correctly. Additionally, it would also appear that the eutectic reaction occurs at 565°C (even lower at Point B, where the cooling rate is high) according to the TC data, whereas it is prescribed to occur at 577°C in the simulation. Unfortunately, the opportunity to further improve the model was greatly undermined by the excessively long execution times of the fully coupled model. It was felt that the level of agreement achieved was sufficiently quantitative to allow exploration of the effect of macrosegregation on liquid encapsulation and hydrogen-based porosity.

**Silicon Segregation Prediction and Comparison to Measured Silicon Distribution** - The predicted distribution of silicon in the wheel near the end of solidification is shown in Figure 5.11. The scale range for mass fraction of silicon is from 0.013 to 0.13. The predicted segregation pattern shows a slight increase in the silicon mass fraction in upper rim and a sharp increase at the rim/spoke junction. A decrease in the silicon mass fraction can be found near the lower rim just
above the rim/spoke junction. The segregation in the hub may be an artifact of the boundary condition imposed at the bottom of the hub and needs further investigation.

The solidification sequence, or pattern, in the wheel for the fully coupled model, is presented below in Figure 5.12 as a series of temperature contours at 5 through 80s. The temperature results are shown as color contours on a plane representing a vertical section through the rim/spoke. The blue colour indicates complete solidification. Contour lines representing fraction liquid equal to 0.99 and 0.5 have been superimposed as black and grey lines, respectively, on the plane section. Note: the liquidus temperature depends on local species content and varies in the fully coupled model.

The solidification path is relatively complex in the wheel. Referring to the 10s contour, complete through-section-thickness solidification begins both approximately $2/3$ of the way up the rim and in the rim flanges (top and bottom). $2/3$ of the way up the rim, the solidification front then moves up toward the upper rim and down toward the rim/spoke junction. In the inboard rim flange, the solidification front moves downward where it meets the front moving up the rim. In the outboard rim flange, solidification moves inward from the outboard rim flange, where it meets the solidification front moving down the rim and then across the spoke and ends in the hub. The formation of two closed, grey-line loops - see 10 and 30s contours - indicates that pockets of material above $0.5 f_l$ are encapsulated at the top of the rim, at the rim/spoke junction and in the hub. Depending on the subsequent evolution of solid fraction in adjacent areas, these areas could potentially result in a significant drop in pressure as they become isolated from a source of liquid to offset the solidification density change. As a reminder, it is important to note that FLUENT is unable to account for the evolution in pressure in an entirely isolated pocket of liquid as mass continuity is applied throughout the domain – see section 4.5 in Chapter 4.
Conceptually, during solidification, silicon is rejected from the solidifying regions into the remaining liquid due to the low solubility of silicon in the $\alpha$-aluminum phase. In the absence of bulk flow, this leads to a gradual increase in the concentration of Si in the inter-dendritic liquid as solidification proceeds. Meanwhile, the density variation between the liquid and solid phases pulls liquid toward areas undergoing solidification. Thus, silicon enriched liquid can be pulled toward regions that are relatively slow to solidify, resulting in a slight increase in the mass fraction of silicon in the upper rim and a more substantive increase at the rim/spoke junction. Alternatively, it can be seen from Figure 5.11 that there is a region deplete in silicon formed directly above the area of liquid encapsulation at the rim/spoke junction. This is a result of enriched liquid being removed from that region to feed the area of liquid encapsulation (referring to the 20s contours in Figure 5.12), resulting in a net, overall, reduction in silicon in the final solid.

![Si Mass Fraction Contour](image)

$C_{\text{Si}}^{\text{initial}} = 0.07$

Figure 5.11 Silicon mass fraction contour predicted by the model at 72s
Prior to showing the comparison between measured and predicted silicon mass fraction in the wheel, it is appropriate to explain how the overall mass fraction of silicon, $C_{Si}$, was estimated from the images taken of the microstructure. The solidified structure of an A356 alloy is nominally comprised of approximately 50% volume fraction primary $\alpha$-aluminum with the balance comprised of Al-Si eutectic. The $C_{Si}$ after solidification can be calculated from:
where $C_{Si,\alpha}$ is the mass fraction of silicon in the primary phase, which can be estimated from the mean of $kC_0$ (0.13*7wt.% and the maximum solubility of Si in $\alpha$ ($C_{Si,\alpha}^{\text{Max}}$ =1.65wt.%), $C_{Si,eut}$ (12.6wt.%) is the eutectic mass fraction of silicon and $f_E$ is the volume or area fraction of the Al-Si eutectic. Thus, the Equation 5.3 can be rewritten as:

$$C_{Si} = C_{Si,\alpha}((1-f_E) + C_{Si,eut}f_E)$$

Equation 5.3

The eutectic area fraction can be calculated using the following procedure:

Step 1 – referring to the micrograph as shown in Figure 5.13 (Left), the image is first converted into a white and black binary image (negative) as shown in Figure 5.13 (Right) in ImageJ, where the region in black represents the primary phase, the rest in white shows the eutectic.

Step 2 - Then $f_E$ is computed from:

$$f_E = \frac{\sum A_{\text{white}}}{\sum A_{\text{black}} + \sum A_{\text{white}}}$$

Equation 5.5

where $\sum A_{\text{white}}$ and $\sum A_{\text{black}}$, respectively, represents the total area of the eutectic and the primary phase. Recently, M.Ghods et al.[63] conducted a sensitivity to the assumptions made in deriving Equation 5.4. The author concluded that application of Equation 5.4 overestimated the volume/area fraction of eutectic and proposed an alternative equation of the form shown in Eq. 5.6[63].

$$C_{Si} = 11.6f_E +1.094$$

Equation 5.6

The uncertainty in $C_{Si}$ by applying Equation 5.6 was estimated to be ±0.28wt.% silicon when

$C_{Si}^{\text{initial}} = 7\text{wt.\%}$.
Figure 5.14 shows a series of images of the as-cast microstructure taken in the vicinity of the spoke/rim junction in the area predicted by the model to have a high level of Si-segregation – see right-hand side images, which show the model predictions. The series of six images were taken from the top of the spoke to the bottom (#1 at 20mm (top), #6 at 0mm (bottom)) of the selected region. In each micrograph, the lighter phase is the primary $\alpha$-aluminum and the darker phase is the eutectic, prior to conversion to a negative black and white binary image. (Note: the alloy has been modified with strontium). Following conversion, the light grey ($\alpha$) becomes black and the dark grey (eutectic) becomes white. The area fraction of primary $\alpha$-aluminum and eutectic in these images was estimated using image analysis. As can be seen, the samples at the top and bottom of the spoke show an ~70:30 split between the area fraction that is primary $\alpha$-aluminum and eutectic, respectively, while towards the centre of the spoke this ratio is reversed as there is ~30:70 split between primary-aluminum and eutectic. These area fractions can be used to estimate the local overall mass fraction of silicon according to Equation 5.6.

The area fraction results for mass fraction of Si together with the model predictions are shown in Figure 5.15. The model profiles of an overall mass fraction of silicon have been extracted along the 3 lines. The horizontal error bars on the data points represent the estimated error in the location of the metallographic sample and the vertical error bars are the estimated error in mass.
fraction assessed by calculating the mass fraction in regions directly adjacent to where the images were taken. The predicted silicon concentration ranges from 6.5\(\text{wt.}\%\) to around 11\(\text{wt.}\%\), whereas the measurement results show a range from 5.5\(\text{wt.}\%\) to 11\(\text{wt.}\%\), as shown in Figure 5.15. Overall, the results show relatively good agreement in terms of the range of mass fraction. However, as seen from micrographs, the maximum silicon concentration is found in the middle of the selected region, whereas the model predicts that the maximum lies closer to the top of the spoke. This discrepancy could be related to the behaviour of the interfacial heat transfer between the wheel and the top die and wheel and the bottom die in this region. The degree to which the distribution is sensitive to the interfacial heat transfer in these regions remains to be determined. At any given point in the cross-section, the maximum difference between the predicted and the measured weight percent is approximately 30\%. 
Figure 5.14 Microstructure along the centre line in the wheel (left) and Location on wheel where comparison was made (Right).

Figure 5.15 Comparison between experimental data (dots) and simulated (lines) silicon mass fraction in the wheel.
Figure 5.16 Microstructure in the rim (left) and location on wheel where comparison were made (Right)
The left-hand-side image in Figure 5.16 shows the as-cast microstructures taken at discrete locations in the middle of the rim. The locations are shown in the right-hand side image (see black crosses), overlaid on a contour of the model predicted Si-segregation in the rim. As can be seen, the samples show a ~70:30 split between the area fraction that is primary \( \alpha \)-aluminum (lighter phase) and eutectic (darker phase). The top micrograph shows a slightly large amount of eutectic relative to the middle and bottom positions. Area fractions extracted from these images have been used to estimate the local overall mass fraction of silicon according to Equation 5.6. The area-based analysis yielded 6.3 wt% for the top, 5.28 wt.% for the middle and 5.27 wt.% for the bottom. Qualitatively, the model predicts the same trend – i.e. very little segregation in this area and a trend to increasing segregation toward the top. Quantitatively, comparing the two sets of results, the model predicts amounts of 7.0, 6.92 and 6.89 wt.%, from top to bottom, respectively, slightly higher than measure from the area analysis.

Figure 5.17 compares the solidification sequence in the wheel, predicted by both the thermal-only (top) and fully coupled (bottom) models at 10, 20, 40 and 50 s. Again, the temperature results are shown as color contours on a plane representing a vertical section through the rim/spoke. Contour lines representing liquid fractions equal to 0.99 and 0.5 have been superimposed as black and grey lines, respectively, on the plane section. The liquidus temperature is fixed in the thermal only model, whereas the liquidus temperature depends on local species content and is varied in the fully coupled model. Comparing the two figures, it is clear that macrosegregation is predicted to have an effect on the volume enclosed by the grey 0.5 \( f_l \) contour line, which would, in turn, determine how much shrinkage porosity may be expected to occur. Generally, there is a reduction in the predicted volume of encapsulated liquid in the fully coupled model.
Porosity Prediction - In this section, the updated porosity model has been applied to predict the porosity size distribution at discrete locations in the commercially produced A356 wheel. As introduced in Chapter 3, the porosity model is sequentially tied to the FLUENT model. The input for the porosity model consists of the local evolution of pressure, temperature, hydrogen concentration in the liquid and liquid fraction/solid fraction.

To begin, the pore size distribution at selected locations is characterized based on the X-ray microtomography data. Following this, the predicted pore size distribution is then compared against experimental data to provide validation of the porosity model.

Historically, pore morphology in metallurgical samples has been characterized by means of optical examination of metallographic samples. The drawback of this approach is that it provides only 2-D information. As a consequence, the porosity area fraction and pore size distribution may be under or overestimated in the case of pores exhibiting a tortuous 3-D morphology - i.e. pores that form at high $f_i$ and have had their growth impacted by the dendrites. In this study, the x-ray microtomography (XMT) analysis technique was applied to provide a 3-D characterization of
porosity with a resolution on the order of a 5-10 μm. This 3-D characterization technique offers improved accuracy regarding to the pore size distribution in the sample.

Figure 5.18 (a) shows the sample locations extracted from the wheel that were X-rayed to quantify the porosity content. Figure 5.18 (b) shows a contour of the hydrogen mass fraction distribution in the wheel cross section predicted by the FLUENT model near the end of solidification. Locations 9T, 9B and 4B, showed the highest volume of porosity in the samples examined and therefore were chosen for analysis with the porosity model. Location 5BT was also chosen for analysis with the porosity model as it is adjacent to the area with the largest degree of hydrogen concentration increase due to macrosegregation. The locations for analysis with the pore model are indicated by the black dots on the contour. Notes: 1) the local hydrogen concentrations predicted near the end of solidification at these locations appear below the contour image; 2) the initial hydrogen concentration, which is estimated, is presented adjacent to the legend; and 3) the samples for x-ray analysis were taken from a wheel following rough machining and, as indicated by the rim cross section and profiles of the inboard and outboard rim flanges. Based on the predictions of the segregation analysis, locations 9B and 5BT are enriched in hydrogen and locations 9T and 4B, where predicted to have approximately the same concentration as the initial liquid – i.e. no net macrosegregation.
Samples from Rim:
Sample 6-9

Samples from Spoke:
Sample 1-5

Figure 5.18 Sample locations (a) and hydrogen mass fraction contour (b) predicted by the model at 72s

The XMT images presented in this study were scanned in Rutherford Appleton Laboratory, Harwell Oxford, United Kingdom. Two scans on ten samples (refer to Figure 5.18 (a)) at discrete locations along the rim/spoke were performed. Each scan was comprised of 2000 slices with a voxel size of 5.916 μm, 6.34 μm or 9.8 μm. Note: that pores with size less than 20 μm were not analyzed – i.e. pores with less than 27 voxels (3×3×3 cube), ~ 20 μm in radius. The image processing was undertaken using ImageJ. To separate the porosity from the metal phase in each XMT image, a suitable greyscale threshold in ImageJ is required. Figure 5.19 illustrates the effect of the threshold value on the XMT images. Too large a greyscale threshold results in non-porosity white spots in the binary images (blue circles), whereas too small a greyscale threshold leads to a reduction in pore size – see series of red circles showing the behaviour of the actual pore(s).
In addition, in some instances, it was noted that in ImageJ, a single pore with a complex, tortuous morphology, may be interpreted as a number of discrete pores. To attempt to address this, the ‘Dilate’ filter was first applied 10 times, followed by ‘erode’ filter 10 times prior to quantifying the porosity size distribution. The effect of above filter combination on image processing is shown in Figure 5.20. As can be seen, the number of small pores decreases and the maximum pore radius increases after applying the filter combination (refer to the bar chart at the bottom). Taking a closer look, the filter combination cannot only combine isolated pores into a single pore (red circles on the 2-D binary image) to increase the interconnectivity but also retain pore size (blue circles on the 2-D binary image) to avoid an artificial increase in pore size. Comparing the 3-D rendered images, it clearly shows the pore clusters in the green circles are now interpreted as individual pores instead of a group of smaller pores. In addition, the total porosity volume fraction slightly increased from 0.55% to 0.6%, also indicating an increase in interconnectivity between pores. As a compromise, the experimental data at all locations was obtained by applying a threshold value of 65 and the ‘Dilate’ and ‘Erode’ filter combination. The pore size was quantified by measuring the equivalent radius of a spherical pore with the same volume. With this procedure, the porosity size distribution at all locations can be obtained.
Figure 5.19 The XMT analysis process
Figure 5.20 Effect of ‘Dilate’ and ‘Erode’ filter combination on image processing
Porosity Characterization

Figure 5.21 shows a 3-D rendering of the porosity at the locations shown in Figure 5.18 (a). All of the locations examined show some porosity; however, locations 4B, near the rim/spoke junction, and 9T, near the top of the rim, clearly show the largest amount. Both locations are adjacent to the areas of 0.5 \( f_i \) encapsulation and are predicted to be slightly enriched in hydrogen - see Figure 5.17 and Figure 5.18 (b). They do not show large pores typical of shrinkage dominated pore formation.

Most of the pores shown in the XMT images are tortuous in appearance and appear to have formed at a late stage in the solidification process, which is consistent with the fact that the metal is continuously degassed and that the initial hydrogen content is likely to be low (although not measured).
The adjustable parameters $A$, $s_{s0}$ and $\sigma$ in the equation describing the nucleation kinetics (Equation 4.22) need to be determined by fitting with experimental data. Among the locations examined, 9B, is best matched to the conditions in the original model[46] – i.e. no liquid encapsulation – and therefore, the experimental data at 9B was used to tune the adjustable parameters in the nucleation kinetics expression. A trial-and-error method was adopted to arrive at a set of nucleation parameters that gave the best fit for location 9B. Figure 5.22 shows the difference in expressions describing nucleation kinetics between the original study[46], on which the porosity model was based, and the current work. The blue curve represents the nucleation site distribution used in reference[46] while the red curve shows the nucleation site distribution used.
in current study. The best fit to the experimental data at location 9B was achieved by assigning $A = 0.3 \text{mm}^{-2}$, $ss_0 = 2.0 \text{mol/m}^3$ and $\sigma = 0.4 \text{mol/m}^3$. Based on the comparison shown, in the current work, the number of nucleation sites activated as a function of hydrogen supersaturation is lower than in the previous work. This difference may be related to holding furnace design and the use of a filter in the sprue, both of which could reduce the number of oxide inclusions entering the die cavity [65] and consequently the population of the nucleation sites available for pore nucleation. Additionally, the average hydrogen saturation $ss_0$ is slightly increased from 1.7 to 2.0, indicating it is more difficult for a gas cavity to form on solid substrates. The reason for this difference is unclear and may be related to small variations in the alloy composition relative to the original study.

Having fit the pore model to the experimental data at location 9B, the model was then used to predict the pore size distributions at location 9T, 4B and 5BT using the same nucleation parameters.

![Figure 5.22 Pore nucleation site distribution](image)

**Figure 5.22 Pore nucleation site distribution**
Figure 5.23 shows the 3-D rendering of the pores (LHS) and the corresponding predicted and measured pore size distributions (RHS), binned in 10-μm increments, at locations 4B, 9T, 9B and 5BT, with the critical solid fraction for mass feeding set to 0.9. The measured data are shown as the yellow bars and the predicted results as the red bars. The cooling rate at each location was added to each plot for reference. Overall, the results show good qualitative agreement in that the model is able to correctly predict the trends with respect to the size distribution range and number density range at the various locations examined, which represent a relatively broad range of solidification conditions. Taking a closer look, the results for locations 9T and 9B show relatively good agreement in terms of the trend of porosity size distribution (again 9B was used to tune the nucleation kinetic parameters). Note: the increase in predicted pore size as the cooling rate is decreased from 9.59 K/s at location 9B to 3.7 K/s at location 9T (more time for hydrogen to diffuse from the bulk to the pore/liquid interface). Additionally, pores at location 9T form and grow in an area of lower pressure, thereby increasing both local supersaturation and pore volume.

The results for location 4B, in contrast, clearly show that the model underpredicts the number density of small pores (< 40μm) in comparison to the XMT data. It is interesting to note that in the 3D rendered image, there are clearly what appears to be a large number of tortuous pores at location 4B in comparison to locations 9B and 9T. Thus, the discrepancy between model and measurements at this location may lie in the processing of XMT the data. In the image processing of the tomography data, it proved difficult to distinguish between the small pores (2 or 3 pixels), suspected to represent areas of interconnectivity in larger tortuous pores and discrete isolated small pores. As a result, many isolated smaller pores remained in the sample and could not be removed.
At location 5BT, the model over-predicted the porosity number density of large pores greater than 20-40μm. Both the pressure drop and hydrogen concentration in the liquid are higher at location 5BT (see Figure 5.24 and Figure 5.25), which explains the tendency to produce large pores based on both mechanisms of pore growth. The reason for the inconsistency with the measured data is unclear and could be due to an error in the ability of the model to predict the evolution in temperature, pressure drop and/or hydrogen concentration at this location in the casting.
Figure 5.23 3-D characterization of porosity (Left) and comparison between measured and predicted pore size distribution at location 4B, 9T, 9B and 5BT (Right)

There are potentially three contributors to the evolution of pore size: 1) hydrogen segregation, as it impacts on the driving force for mass transfer; 2) pressure drop, as it impacts on both the driving force for mass transfer and pore volume (the latter dominant at $f_s > 0.9$ where shrinkage based pore growth occurs); and 3) cooling rate, as it impacts on the time for mass transfer to occur at $f_s < 0.9$.

To explore the role of various contributor to pore growth, the evolution in the liquid concentration of hydrogen, the evolution in the pressure and the cooling rate has been plotted for the locations examined with the model. Figure 5.24 plots the variation in $C_{H,liq}$ with $f_s$; Figure 5.25

134
plots the variation in pressure with $f_s$; and the average cooling rates at four locations during solidification are included in Figure 5.23.

Focusing first on the evolution of $C_{H,liq}$, Figure 5.24, both a full $f_s$ range, plot (a), and an expanded image for $f_s < 0.6$, plot (b), are provided. The expanded image better shows the evolution in $C_{H,liq}$ over the range of $f_s$ where $C_{H,liq}$ is input to the porosity code from FLUENT rather than calculated from Scheil approximate (Equation 4.27). Recall the evolution of the composition of the liquid is calculated in FLUENT only up to the eutectic reaction. Given the data were shown, the evolution in $C_{H,liq}$ with $f_s$ is relatively consistent among the four locations examined with only relatively small differences. The $C_{H,liq}$ at a given $f_s$ at location 5BT is highest followed by location 4B, 9T and 9B, consistent with the contours of the predicted Si segregation shown earlier. Based on the parameters in nucleation kinetics expression, the average supersaturation ($ss_0$) for pore nucleation in the current model is $2.0 \ mol/m^3$. Comparing this with the plots shown in Figure 5.24, it would appear that nucleation occurs at $f_s$’s in excess of 0.8, or at relatively high solid fractions.

As can be seen from Figure 5.25, the local pressure evolution at the various locations examined is significantly different. All show an abrupt drop in pressure reaching a minimum of -18,000 to -24,000 Pa. However, the range of solid fractions at which this occurs varies from approximately 0.3 to 0.9, depending on location. Additionally, location 9T shows an increase in pressure after reaching the minimum at approximately $0.5 f_s$, whereas the other three locations do not exhibit a pressure rise. Moreover, the pressure drop at locations 5BT and 9B occurs at $f_s$’s approximately consistent with when the eutectic transformation occurs, whereas the pressure drop at location 9T and 4B are very different – 9T occurring at an $f_s$ of ~0.3 and 4B at an $f_s > 0.9$. The reason for the difference in behavior between the various locations is unclear. One hypothesis is that 9T and 4B are at locations associated with some liquid encapsulation, where the pressure drop
may be driven by the loss of feeding associated with encapsulation, whereas 9B and 5BT occur in locations that do not indicate liquid encapsulation and therefore the pressure evolution may be more related to an abrupt change in the solidification rate associated with eutectic formation.

Finally, comparing cooling rates, in order of decreasing cooling rate, location 9B has an average cooling rate of 9.59 K/s; 9T, 3.7 K/s; 5BT, 1.45K/s; and 4B 1.35K/s.

Given the differences in \(C_{H,liq}\), pressure and cooling rate described above between the different locations examined and the porosity observed (predicted and measured) it would appear that the evolution in pressure has the dominant effect on pore growth, but only under conditions where pores have nucleated prior to the pressure drop - i.e. at location 4B. Otherwise, the cooling rate appears to have the dominant effect, which explains why 9T produces more porosity than 9B in spite of the pressure increase toward the end of solidification. Location 5BT is predicted to produce more porosity than 9T and 9B, because of the lower cooling rate and potentially also because of the slightly higher hydrogen content. The significant pressure drop predicted at 5BT occurs before pore nucleation and hence does not have a significant impact. The reason for the large discrepancy observed between the model predictions and XMT measurements at 5BT is still, however, not clear.
Figure 5.24 Hydrogen concentration in liquid as a function of solid fraction at location 4B, 9T, 9B and 5BT; (a) full range in $f_s$, (b) expanded view up to $f_s = 0.6$. 
To assess the effect of the critical solid fraction on pore growth based on pressure drop, a sensitivity analysis was performed for location 4B. Depending on the microstructure at the locations of interest, the shrinkage driven mechanism might take place at various solid fractions. The base critical solid fraction was set to 0.9, identical to previous cases. The critical solid fraction was varied from 0.8 to 1.0 in increments of 0.05. With a value of 1.0 representing the case where the porosity model does not switch to a shrinkage-based evolution in porosity. All of the other model parameters were held constant. The resulting predicted pore size distribution, binned in 10-μm increments, at locations 4B are shown in Figure 5.26, along with measured (experimental) data.
The number at the end of each legend denotes the critical solid fraction adopted for each case. The results indicate that the pore size distribution at 4B is strongly affected by choice of the critical solid fraction. The lower the critical solid fraction, the larger the number of small pores predicted. For instance, the porosity number density in the 30-40μm bin increases from 0.008 to 0.128 as the critical fraction decreases from 0.9 to 0.85. A lower critical solid fraction also significantly reduces the maximum pore size – e.g. a maximum pore size of 90μm is predicted for a critical $f_s$ of 0.8 verses 150μm for $f_s = 1$ (no shrinkage-based pore growth). Overall, the pore size distribution shifts towards small pores. It would appear, therefore, that the original formulation of the hydrogen porosity-based model that applied mass-transfer based pore growth over the entire solidification range overestimates pore growth.
6 Summary, Conclusions and Future Work

Summary

This research focused on developing a methodology to investigate hydrogen macrosegregation during solidification of aluminum alloy A356 and its impact on hydrogen-based pore formation. The goal was to successfully implement the methodology to predict pore size distribution at discrete locations in a low-pressure, die cast, automotive wheel. Toward this goal, the work focused on the development of a user-defined subroutine (UDS) run within ANSYS FLUENT 16.0 capable of calculating hydrogen macrosegregation. This methodology was referred to as the UDS method throughout the thesis. The proposed UDS method was initially implemented in a 2-D axisymmetric, geometrically simplified, L-shape casting. The UDS method for hydrogen segregation was verified by first formulating a version of the UDS for Si-segregation and then comparing the predictions with the “built-in” ability of FLUENT to calculate alloy species segregation. In addition, Si-segregation in the wheel was verified by comparing 3-D model prediction with the measurement of samples taken from the rim/spoke junction.

The evolution in liquid fraction, temperature, pressure and hydrogen concentration in the liquid predicted by FLUENT at a specific location, was extracted and then fed into a previously developed hydrogen porosity model[46] (recoded in Python 2.7.1) to predict the pore size distribution. The porosity model was also modified to include a two-stage pore growth formulation to account for pore growth at high $f_s$, where mass feeding can no longer occur. Using the L-shaped casting, a sensitivity analysis was performed to investigate the impact of various numerical and process parameters on some of the key predictions of the FLUENT model and hydrogen porosity
model. A key focus of the sensitivity analysis was to explore the relative contribution of hydrogen segregation, pressure evolution and cooling rate on pore nucleation and growth.

The FLUENT model, with the UDS method to predict hydrogen segregation, was then applied to simulated the evolution of temperature, $f_i$, hydrogen concentration in the liquid and pressure in an LPDC wheel and then to simulate the evolution of porosity at discrete locations in the wheel using the updated porosity model. Finally, the predictions of the updated porosity model were compared to XMT measurements of the pore size distribution at specific locations in the wheel casting and the relative contribution of hydrogen segregation, pressure evolution and cooling rate in pore growth were assessed in the wheel casting.

**Conclusions**

1) It is proposed that the UDS method is capable of characterizing hydrogen segregation during wheel solidification in the low pressure die casting (LPDC) process. In addition, FLUENT is computationally efficient to simulate the local evolution in pressure and temperature with respect to $f_i$ for the calculations in the porosity model. Whereas FLUENT has limitations in solving pressure evolution in the area of encapsulation and struggles with Darcy flow at high solid fraction (The velocity attenuation parameter $A_{mush} (kg/m^3.s)$ in the current FLUENT model was limited to 1E7 due to numerical convergence issue).

2) The computational domain of the LPDC process was based on a five-spoke wheel. The FLUENT thermal model had been demonstrated to be able to qualitatively describe the temperature evolution in both the wheel and die sections. Comparisons showed the maximum difference of 35°C between the thermocouple measurements and the simulations in the majority of examined locations. It also demonstrated that the interfacial heat transfer coefficients between
wheel and various die components could significantly affect FLUENT model capability to accurately describe temperature evolution in the wheel;

3) The fully-coupled FLUENT model demonstrated the capability to qualitatively describe species macrosegregation resulting from solidification shrinkage induced fluid flow. And the rim/spoke junction was identified as a key area for species enrichment;

4) The 3-D XMT analysis of the pore size distribution at various locations in the wheel showed the spoke section in the vicinity of the rim/spoke junction and top rim were critical areas for microporosity formation. The parameters in nucleation kinetics were derived by fitting measured data, showing increased difficulties for pore nucleation due to a reduction in the number of oxides (filter) and initial hydrogen content in the melt (degassing). The current model indicates a large amount of pores was nucleated at a relatively high solid fraction (around 0.8);

5) The resulting pore size distribution was binned in 10-μm increments. The key factors affecting pore growth include local hydrogen segregation, pressure evolution and cooling rate. Higher hydrogen content can increase hydrogen mass transfer rate, resulting in greater pore size. The evolution in pressure has the dominant effect on pore growth, but only under conditions where pores have nucleated prior to the abrupt pressure drop. Otherwise, the cooling rate appears to have the dominant effect. The model prediction shows pore size increases with decreasing pressured drop and cooling rate. However, switching to shrinkage based pore growth mechanism at high solid fraction (~0.9) impedes pore growth. As a result, the amount of small pores increases with decreasing critical solid fraction.

**Future Work**

The FLUENT model adopted in current work did not consider die cavity filling, resulting in an initial temperature of the wheel domain deviate from the measurement data. Additionally,
the errors in the thermal boundary conditions, more specifically the interfacial heat transfer at the wheel/die interfaces critically affected the model capability of describing temperature evolution in the wheel, and in turn would affect the species macrosegregation.

In order to correctly describe the temperature evolution in the wheel during an LPDC process, the approximation of cavity filling and more accurate interfacial heat transfer coefficients—i.e. include impacts of wheel deformation and gap formation—are required.

The microporosity model[46] was applied to predict pore size distribution in an LPDC aluminum alloy wheel. In order to correctly describe pore growth, the accurate simulation of pressure drop is required. A second dendrite arm spacing (SDAS) related velocity attenuation parameter $A_{mush} \ (kg/m^3.s)$ should be applied in the FLUENT model to improve model accuracy regarding to prediction in pressure evolution.
References


Appendix

As described in Chapter 4, the user defined scalars (UDSs) and corresponding user defined functions (UDFs) were applied to solve for the Hydrogen macrosegregation during solidification.

The source code for the UDFs are given below.

### Source code for the UDFs

<table>
<thead>
<tr>
<th>UDS</th>
<th>Accumulation Term</th>
<th>Source Term</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>UDS0</strong></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

```c
#include "udf.h"
#include "mem.h"

DEFINE_UDS_UNSTEADY(my_uds_hgasunsteady,c,t,i,apu,su)
{
    real physical_dt, vol, rho, phi_old,phi_old_yi;

    physical_dt = RP_Get_Real("physical-time-step");
    vol = C_VOLUME(c,t);
    rho = C_R_M1(c,t);
    phi_old = C_STORAGE_R(c,t,SV_UDSI_M1(0));
    phi_old_yi = C_STORAGE_R(c,t,SV_UDSI_M1(3));

    if(phi_old<=0.126)
    {
        *apu = -rho*vol/
            physical_dt;/*implicit part*/
        *su = rho*vol*phi_old_yi/
            physical_dt;/*explicit part*/
    }
    else
    {
        *apu = rho*vol/
            physical_dt;/*implicit part*/
        *su = -rho*vol*phi_old_yi/
            physical_dt;/*explicit part*/;
    }
}
```

```c
#include "udf.h"
#include "mem.h"
#define k 0.069
#define delt 0.001

DEFINE_SOURCE(uds_source_hgasliq,c,t,ds,i)
{
    real physical_dt,source,phi_old,slf_old,slf_curr,
        lqf_old=C_LIQF_M1(c,t);
    real lqf_curr=C_LIQF(c,t);
    real yliq=C_UDSI(c,t,2);
    slf_old = 1-lqf_old;
    slf_curr = 1-lqf_curr;
    phi_old = C_STORAGE_R(c,t,SV_UDSI_M1(0));
    hliq_old = C_STORAGE_R(c,t,SV_UDSI_M1(3));

    if(phi_old<=0.126)
    {
        source =
            -k*hliq_old*(2685.0*slf_curr-
                2685.0*slf_old)/physical_dt+(2685.0*slf_curr*
                yliq-2685.0*slf_old*hliq_old)/physical_dt;
        ds[i] = -k*(2685.0*slf_curr-2685.0*slf_old)/physical_dt;
    }
    else
    {
        source = 0.0;
        ds[i] = 0.0;
    }
    return source;
}
```
UDSI

```c
#include "udf.h"
#include "mem.h"

DEFINE_UDS_UNSTEADY(my_uds_hgasunsteady,c,t,i,apu,su)
{
    real physical_dt, vol, rho,
    phi_old, phi_old_yi;

    physical_dt = RP_Get_Real("physical-time-step");
    vol = C_VOLUME(c,t);
    rho = C_R_M1(c,t);
    phi_old = C_STORAGE_R(c,t,SV_UDSI_M1(0));
    phi_old_yi = C_STORAGE_R(c,t,SV_UDSI_M1(3));

    if(phi_old<=0.126)
    {
        *apu = -rho*vol/physical_dt;/*implicit part*/
        *su = rho*vol*phi_old_yi/physical_dt;/*explicit part*/
    } else
    {
        *apu = rho*vol/physical_dt;/*implicit part*/
        *su = -rho*vol*phi_old_yi/physical_dt;/*explicit part*/;
    }
}
```

```
#include "udf.h"
#include "mem.h"
#define k 0.069 /*hgas partition coefficient*/

DEFINE_SOURCE(uds_source_hgas,c,t,ds,i)
{
    real source, physical_dt;
    real lqf_old=C_LIQF_M1(c,t);
    real lqf_curr=C_LIQF(c,t);
    real slf_old;
    real slf_curr;
    real phi_old;
    real yliq=C_UDSI(c,t,2);
    real hliq_old = 1-lqf_old;
    real hliq_curr = 1-lqf_curr;
    real phi_old = C_STORAGE_R(c,t,SV_UDSI_M1(0));
    real hliq_old = C_STORAGE_R(c,t,SV_UDSI_M1(2));
    physical_dt = RP_Get_Real("physical-time-step");

    if(phi_old<=0.126)
    {
        source = k*slf_old*2685.0*(slf_curr-slff_old)/physical_dt+2540.0*(yliq-hliq_current*lqf_old)/physical_dt;
        ds[i]=0.0;
    } else
    {
        source = ds[i]=0.0;
    }

    return source;
}
```