**Finite Element Analysis of Flow and Heat Transfer
of Molten Metal During the Slow Shot of Die Castings**

by

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A thesis submitted to

the Faculty of Graduate Studies and Research

in partial fulfillment of the requirements for the degree of

Doctor of Philosophy

Department of Mechanical and Aerospace Engineering

Ottawa - Carleton Institute for Mechanical and Aerospace Engineering

Carleton University

Ottawa, Canada

April, 2004

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ISBN: 0-612-97854-0

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ISBN: 0-612-97854-0

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Thesis Supervisor

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Abstract

The aim of this thesis is to investigate the flow and heat transfer of molten metal in the shot sleeve of a cold-chamber die casting machine during the slow shot. A coupled fluid flow and solidification model is developed to predict the plunger profile that will produce the desired wave dynamics to minimize air entrapment and the amount and distribution of solidified phases in the shot sleeve.

A three-dimensional (3-D) finite element method was proposed for the numerical simulation of the fluid flow and heat transfer. The analysis was conducted by solving a coupled problem governed by the conservation of mass, momentum and energy. Simo's version of Newmark algorithm was implemented to solve the momentum equation. The corresponding software was developed and verified using well known test problems for fluid flow and heat transfer. The computed predictions were compared with experimental results. The present method is based on a Lagrangian finite element formulation whereby the fluid is discretized into volume elements that deform due to the movement of the plunger. When the deformation of elements becomes large, remeshing is done, and the data is mapped from the badly-deformed mesh to a new improved mesh.

Since the critical slow shot velocity has an important influence upon the flow pattern and wave formation of molten metal, the effects of inner diameter of a shot sleeve, plunger acceleration, and initial fraction filled on the critical slow shot velocity

are investigated. The results are valuable since data acquisition in the shot sleeve is difficult.

In the cylindrical shot sleeve plunger velocities greater than the critical slow shot velocity with initial fraction filled of 0.5 cause the wave front to roll over and break at the ceiling of the shot sleeve, and entrap air. With the initial fraction filled of 0.3 the wave will break at both sides of the sleeve before the wave reaches the ceiling. Plunger velocities slower than the critical velocity do not create a full height wave which leads to the air entrapment in front of the plunger.

The coupling between the flow and heat transfer of the molten metal gives a better picture of the fluid in a shot sleeve. On one hand, the velocity field attained by the fluid flow analysis advects the enthalpy for the heat transfer analysis. On the other hand, the heat transfer analysis solves the enthalpy, temperature and fraction solid fields which consequently determine the density and viscosity fields for the fluid flow analysis. The analysis for the cylindrical shot sleeve found that the solidification of molten metal does happen during the slow shot of die castings although the solidification only occurs near the plunger which may not have a big effect on the following fast shot process.

To my wife,
my parents,
and my daughter, Yifan

Acknowledgments

I would like to thank Dr. John A. Goldak, my supervisor, for his invaluable guidance and financial support; Dr. Edward Hughes for his guidance with the mathematics and teaching me the real meaning of clarity; Mr. Dan Downey for his computer system support; Mr. Stanislav Tchernov and Mr. Shaodong Wang for their part of software development.

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Chapter 1

Introduction

The goal of any manufacturing industry is to minimize the processing steps to produce a final product, i.e., if possible a one-step process from raw material to final product. Accomplishing this goal is termed net shape manufacturing. Die casting in horizontal cold-chambers is currently the most common process for manufacturing near-net shape cast components of aluminum and magnesium alloys. It allows very high production rates with close dimensional tolerance and an excellent surface finish.

1.1 Die Casting in Cold-Chamber Machines

There are two types of die casting machines – ‘Hot-Chamber’ and ‘Cold-Chamber’ die casting machines. For alloys of low melting-point, up to and including the widely-used zinc alloys, it is possible to employ hot-chamber machines which have an integral

metal-pump immersed in the molten metal. This is not practical with aluminum and copper-base alloys, since the ferrous pump elements suffer erosion by the melt. These higher melting-point alloys are die cast with cold-chamber machines. An illustration of a cold-chamber die casting machine is presented in Fig. 1.1*.

Figure 1.1: Graphical illustration of a cold-chamber die casting machine.

The cycle using the cold-chamber die casting process is shown in Fig. 1.2. Initially, liquid metal is poured into the shot sleeve through the pouring hole (a). The liquid metal is then immediately pushed at a low speed (b) through a runner (c) into a die

*Fig. 1.1 and 1.2 are from http://media.wiley.com/product_data/excerpt/16/04712013/0471201316.pdf.

cavity (d) squeezed under high pressure. High pressures are maintained on the alloy during solidification. After complete solidification, the die opens (e) and the part is ejected (f).

Figure 1.2: Casting cycle for cold-chamber die casting.

Most consider the die casting process to be very complicated and difficult to control. The injection process in particular is difficult to control. A number of

potential problems can occur. One potential problem is that as the liquid metal is poured into the shot sleeve, portions of it might solidify upon striking the shot sleeve wall prior to initiation of the injection process. Oxide can develop on the solidified particles ultimately resulting in defects within the die casting. The most common defect in die casting is porosity, which limits the integrity of the casting. Although there are different mechanisms involved in porosity formation [1], the most important one in die casting is generally thought to be the entrapment of air during the injection process.

To minimize air entrapment, the molten metal injection process usually consists of two phases: slow shot (Fig. 1.2(b)-(c)) and fast shot (Fig. 1.2(c)-(d)). The significance of air entrapment during the slow shot should not be underestimated. It can have a significantly adverse effect on casting porosity. For example, with a cold chamber initially 50% full, there is more air in the cold chamber than in the die cavity and runner system. The research of Lindsey and Wallace [2] clearly proves that air entrapment in the cold chamber can increase porosity. The large amount of entrapped air may even cause interruptions in the flow of metal in the runner due to solidification effects [3].

During the slow shot phase, the plunger should push the metal into the die as fast as possible to avoid premature solidification that could cause incomplete filling (cold shut) or internal defects. However, if the plunger moves too fast, the molten

metal will fold over, trapping air, that may appear as internal defects in the final part. Ideally, the plunger should first force the molten metal to rise and fill the upper section of the shot sleeve, and then move at constant speed until the shot sleeve is completely filled with molten metal. During the plunger movement, a wave forms. The aim of this thesis is

1. to determine the flow pattern and wave formation of molten metal in the shot sleeve to minimize air entrapment;
2. to predict the solidification during the slow shot of the die casting process and its effects on the subsequent fast shot, if solidification does occur;
3. to enable die casting designers to optimize the plunger profile and to improve their overall understanding of the slow shot. The software developed is intended to be used by designers in industry.

1.2 A Review of Experimental and Theoretical Analysis of Fluid Flow During the Slow Shot

To study the effects of plunger velocity on metal wave height in the shot sleeve, Garber [4] developed a theoretical model based on the conservation of mass flow and energy (Bernoulli's equation). By considering the special case where the wave is

assumed to have the same height at the cylindrical cross-section and the total wave height equals the sleeve's inner diameter, Garber derived a formula for the *critical slow shot velocity* of the plunger given the inner diameter of the shot sleeve and initial fraction filled. The critical plunger velocity will produce a wave which just fills the shot sleeve cross-section. This velocity ideally minimizes air entrapment by pushing air ahead of the wave and through the vents in the die (see Fig. 1.3A). Results from Garber's mathematical model and verification through water analogue experiments led to his conclusion that less air entrapment occurs in the shot sleeve when the plunger remains at critical velocity during the slow shot stage of injection. The waves created by plunger velocities below this critical velocity entrap air since a full height wave is not created before the sleeve is full of metal and air is trapped as shown in Fig. 1.3C. Plunger velocities above the critical velocity cause the wave front to curl over and break, entrapping air, as shown in Fig. 1.3B. However, because full consideration was not given to the effects of the plunger's acceleration (i.e., it was only modeled as an instantaneous acceleration to critical velocity), Garber concluded that his model was not able to predict an acceptable value for critical velocity for initial fractions filled lower than 0.5 because the waves that formed were unstable. Garber did mention in the conclusion that a smooth acceleration should be used as the plunger accelerates to the critical speed.

On the other hand, the Bühler Brothers Company [5] developed an injection

Figure 1.3: Schematic sketch of flow in the shot sleeve. (From [10])

system called *Parashot*. Instead of molten metal injection in phases, i.e., slow shot and fast shot with abruptly changing accelerations the plunger moves with a constant acceleration. It was intended to minimize air entrapment in the injection phase.

Based on the above observations, it has been accepted that the acceleration is an important control parameter for maintaining a stable wave front. A series of water analogue experiments have been conducted [6, 7, 8]. In these experimental studies, the plunger velocity increases linearly with the distance traveled, resulting in

an acceleration which grows exponentially with time. That is

$$\frac{dx}{dt} = \alpha x \quad (1.1)$$

where α is a constant of proportionality and

$$x = x_0 e^{\alpha t} \quad (1.2)$$

$$\ddot{x} = x_0 \alpha^2 e^{\alpha t}. \quad (1.3)$$

where x_0 is the plunger position at $t = 0$. The reason for this choice is that the plunger velocity profiles are typically programmed by specifying the plunger velocity as a function of plunger position. In these tests, the amount of entrapped air was measured for a plunger moving at different accelerations in the initial stage. One of the main conclusions of this analysis was that a *best* plunger acceleration does exist for minimum air entrapment. An appropriate acceleration will lead to a wave profile similar to that of Fig. 1.3A. A higher acceleration might lead to wave roll-over and breaking as shown in Fig. 1.3B. If the acceleration is too low, air will be trapped between the incoming wave and the wave reflected from the far end of the shot sleeve which is similar to Fig. 1.3C.

Based upon the experimental results, theoretical works aimed at optimizing the acceleration parameters have been done. Representative mathematical models based on the shallow-water theory can be found in papers by Thome and Brevick [10, 11], Tszeng and Chu [9], and López *et al.* [12, 13]. Some improvements have been made.

For example, a model for plunger motion with time-power acceleration law ($v = \alpha t^n$) was proposed in [12]. Recently, Hernández *et al.* [20] proposed a model which takes into account of wave reflection effects at the far end of the shot sleeve. The theoretical predictions of wave profiles match qualitatively well with the experimental results and the following conclusions can be drawn:

- The acceleration of the plunger plays a very important role in the stability of wave front and therefore the amount of air entrapment.
- A minimum initial fraction filled is required to avoid the wave breaking before the molten metal reaches the shot sleeve ceiling.
- The exponential acceleration produces steeper wave profiles and so requires shorter filling times than the time-power acceleration law.

Although the theoretical papers help provide a better physical understanding of the overall behavior of molten metal in the shot sleeve, they do have their limitations. For example, the shot sleeve is generally cylindrical which is circular in cross section and the flow is symmetrical with respect to the vertical plane of the shot sleeve. The theoretical models only apply to this symmetry plane. It would be difficult to take into account factors such as viscosity variation caused by solidification because the inviscid flow theory is assumed.

1.3 Numerical Analysis of Fluid Flow During the Slow Shot

The numerical simulation of flow problems involving a free surface remains a challenging task in fluid dynamics despite the continuous development of new solution techniques and the advent of powerful computational platforms. The problem becomes particularly difficult in the case of three-dimensional (3-D) transient flows with free surface which is the case for the flow of molten metal in the shot sleeve in a die casting machine. The moving plunger imposes an additional difficulty.

Numerical simulations of fluid flow in the slow shot that have been carried out are scarce. In 2-D analysis, Gómez *et al.* [19] developed a model to simulate the wave breaking in the shot sleeve. A finite difference method (FDM) is employed to discretize the Navier-Stokes equations in a Cartesian grid and the incompressibility is enforced by a projection method. The free surface is captured by a level set method. Hernández *et al.* [18, 20] first established an analytical model of the wave profile based on the shallow-water equations and then solved the equations governing the wave profile numerically using a deformable finite difference grid. The Navier-Stokes equations were solved numerically by the Computational Fluid Dynamic (CFD) program WRAFTS in which the finite element method (FEM) was used for the conservation equations, a volume of fluid method (VOF) was used to describe the evolution

of the free surface, and the mesh was moved and deformed using a technique similar to the Arbitrary Lagrangian-Eulerian method (ALE). The wave profiles computed numerically by these two approaches matched qualitatively.

In 3-D analysis, The same WRAFTS program was utilized by Backer and Sant [14] to simulate the motion of the fluid in a shot sleeve and the effect of plunger acceleration was investigated. Kuo and Hwang [15, 16] used a finite difference method (FDM) to solve the Navier-Stokes equations in which the pressure field was obtained by solving the Laplace's equation. The turbulence viscosity was computed by the $k-\epsilon$ model and was found to be 10^3 - 10^4 times higher than the molecular viscosity. A three-dimensional Cartesian mesh called 'variable spacing even mesh' (VSEM) scheme was used to represent the moving plunger and the SOLA-MAC technique was used for the free surface. The effect of plunger velocity on the flow pattern was investigated but it is not clear what acceleration law was used to reach the maximum plunger velocities. The length of shot sleeve cavity used for the simulation was 20 cm, which is relatively short compared to the normal shot sleeve cavity length of 40-100 cm. Therefore, some phenomena may not be observed at later times of the slow shot. Khayat [17] proposed a 3-D boundary element method (BEM) for the numerical simulation of potential flow in the shot sleeve during the slow shot. An Eulerian front-tracking method (EFTM) which is related to the VOF method was implemented to determine the evolution of the free surface by monitoring the amount of fluid coming out of

and into the volume elements located at the surface. The motion of the plunger was captured by the deformation of the cavity mesh. Laplace's equation[†] was solved for each time step to determine the motion of the fluid.

To summarize the literature four major choices have been made in the simulation of the fluid flow in a shot sleeve:

1. The governing equations – the Navier-Stokes equations and potential flow (Laplace's equation). Most solved the Navier-Stokes equations.
2. The discretization method – the FEM, FDM and BEM.
3. The tracking of the free-surface – the VOF, MAC and level set methods.
4. The motion of the plunger – ALE and VSEM methods.

The major limitations of the published research on wave formation in a die casting shot sleeve can be summarized as follows:

- There is only one simulation of the breaking wave in a shot sleeve by Gómez *et al.* [19] in a 2-D analysis. Three publications [14, 15, 17] describing a 3-D transient analyses were found and none solved for a breaking wave.
- The energy equation was not solved and the effects of solidification on the fluid flow were not considered in any of the published papers.

[†] $\nabla \cdot \mathbf{v}(\mathbf{X}, t) = \nabla^2 \phi(\mathbf{X}, t) = 0$, where $\nabla = (\partial/\partial x, \partial/\partial y, \partial/\partial z)$ is the gradient operator, ∇^2 denotes the Laplacian operator and ϕ is a potential.

- None of the published analyses were in a form that was suitable for use by designers.

1.4 Selection of the Coordinate Systems

In analyzing the fluid flow with a free surface, the primary equations are the Navier-Stokes equations for incompressible flow, i.e., the conservation of momentum equation for a Newtonian fluid and the conservation of mass given by the continuity equation. The energy equation is secondary in the sense that its primary effect on the liquid is to alter viscosity and slightly change density. If the liquid solidifies, then the viscosity of the liquid can change by orders of magnitude and density can increase roughly 6% for aluminum alloys.

There are two coordinate systems that are commonly used in computational fluid dynamics: Eulerian and Lagrangian. Since each coordinate system has its own unique advantages and disadvantages, the choice will depend on the particular application.

The numerical analysis of the fluid flow is usually done in an Eulerian frame. In the Eulerian coordinate system, the mesh remains fixed in space and the identity of individual material points, i.e., fluid elements is not maintained. For a fixed spatial domain, this minimizes the difficulty in meshing. In this approach, the use of fixed structured grids affords simplicity and availability of well-tested, economical field solvers. However, Eulerian methods do have their disadvantages. One of the

challenges is caused by the nonlinear term $\mathbf{v} \cdot \nabla \mathbf{v}$ that makes the system of equations asymmetric and nonlinear. Dealing with free surfaces is also a serious challenge.

The major challenge to the modeling of the free surface has been the ability to track its movement. The most common methods used today are the Marker and Cell (MAC), and Volume of Fluid (VOF). The MAC technique employs a number of massless marker particles placed in the free surface of the fluid to track the motion of the free surface. Although this method is relatively simple, it requires a great deal of computer memory. The VOF method requires minimal storage. It is based on the volume fraction of fluid in each computational cell. The fractional volume has a double function of flagging the cell and reconstructing the free surface. Solution algorithms such as SMAC, SOLA-MAC, and SOLA-VOF have been developed in this area [21, 22, 23]. More recently, level set methods have been developed. These methods add a signed distance or phase field function such that the free surface or interface is the level set or contour on which the distance or phase field function has value zero. This distance or phase field function is advected with the velocity field of the fluid [24].

The use of Arbitrary Lagrangian-Eulerian (ALE) formulations have been shown to be a very useful strategy to circumvent the inherent limitations of both Eulerian and Lagrangian numerical methods. The fundamental idea of the ALE methods is to treat the spatial discretization or mesh as a separate entity, independent of the

spatial domain, as in the Eulerian approach. In this way, the large distortion of the spatial cells (finite elements in our case) appearing in Lagrangian formulations can be avoided and material surfaces, like the boundaries, can be traced more easily. Representative papers on the development of ALE finite element methods are Donea [25], Belytschko *et al.* [26], Hughes *et al.* [27], and Huerta and Liu [28] along with the latest development by Armero and Love [29]. As mentioned in the previous section, an ALE method was also used in the numerical simulation of the wave profile during the slow shot under the operating conditions relatively close to its optimal [20], i.e, it is unlikely that the wave would break. Generally, the wave in the shot sleeve could break, which would lead to a very large distortion of mesh. As Armero and Love stated, the amount of mesh distortion that can be handled by the ALE methods is limited: singular deformation gradients eventually appear when computed from the interpolated fields based on excessively distorted finite elements. A full remeshing of the problem is eventually required to overcome this limit although the ALE methods could delay remeshing.

Usually problems in solid mechanics are more conveniently set in a Lagrangian framework. In the Lagrangian coordinate system, each cell of the mesh that subdivides the fluid contains the same set of material points for all time. The difficulties related to the Eulerian methods disappear. The challenge arises from the mesh management needed to deal with mesh distortion. That is, one has to deal with an ex-

cessive deformation of the material which may lead to a high distortion of the spatial discretization and the breakdown of the computation due to ill-defined interpolations.

The earliest fully Lagrangian treatment of viscous flows may have been advanced by Hirt *et al* [30]. In their pioneering work, Belytschko *et al.* [31] noted the advantages of the Lagrangian formulation for problems of fluid-structure interaction involving large structural deformations. Other noteworthy early works are those of Bach *et al.* [32] and Ramaswamy *et al.* [33, 34]. These approaches are based on a reformulation of the Navier-Stokes equations in material coordinates, which subsequently are updated via an *ad hoc* iterative procedure. However, because these methods were implemented on a mesh with fixed topology, they were limited in the extent of the geometrical effects they could account for. In the past, the main technological obstacle standing in the way of fully Lagrangian finite element methods for fluids has been the lack of automated and adaptive meshing. However, the advances in meshing [36, 37] enable the continuous remeshing of the fluid mass as the flow proceeds, which effectively opens the way to the application of Lagrangian methods. Radovitzky and Ortiz [35] developed a fully Lagrangian 2-D finite element method for the analysis of Newtonian flows based on continuous and adaptive remeshing. The principal advantage of the approach lies in the treatment of boundary conditions at material surfaces such as free boundaries, fluid/fluid or fluid/solid interfaces. In contrast to Eulerian approaches, boundary conditions are enforced at material surfaces *ab initio* and therefore require

no special attention.

Above all, the following advantages can be drawn if the current research is formulated in a Lagrangian frame:

- Allowing a simple formulation of the governing balance equations and the system of equations is symmetric positive definite.
- The free surface problem is relatively easy to solve. In this research it is especially important to determine the location of the free surface with high degree of accuracy.
- Dealing with the moving plunger imposes no difficulty.
- When one deals with a fixed quantity or mass of liquid, the Lagrangian framework would seem more natural.

In addition, several automated meshing tools have been developed in this research group at the Carleton University, which enhance the possibility of the Lagrangian formulation. For these reasons, it was decided to work in a fully Lagrangian framework and conduct the automated remeshing of the fluid mass when necessary as the flow proceeds.

Table 1.1: Definition of dimensionless numbers

Parameter	Definition
Reynolds number	$\text{Re} = \frac{\rho V L}{\mu}$
Froude number	$\text{Fr} = \frac{V^2}{gL}$
Peclet number	$\text{Pe} = \frac{\rho c_p V L}{\kappa}$
Brinkman number	$\text{Br} = \frac{\mu V^2}{\kappa \Delta T}$
Prandtl number	$\text{Pr} = \frac{c_p \mu}{\kappa}$
Weber number	$\text{We} = \frac{\rho V^2 K}{\gamma}$
Grashof number	$\text{Gr} = \frac{\beta \Delta T g L^3 \rho^2}{\mu^2}$

1.5 Dimensionless Analysis

The dimensionless numbers relevant to this thesis are defined in Table 1.1. The power of dimensionless analysis lies in the fact that these dimensionless numbers are able to characterize a system.

A dimensionless number is important exactly when it is an invariant of a symmetry group of the governing equation of the problem. For example, the Reynolds number is an invariant of a symmetry group of the Navier-Stokes equations. The *Reynolds number* represents the ratio between the inertial and viscous forces. In Table 1.2, where the approximate values of the material properties for pure aluminum and some

Table 1.2: Dimensionless numbers of molten aluminum through narrow pipe. The values are approximately equal to values for the shot sleeve analysis in this thesis.

Density (ρ)	2500 kg/m ³	Re	125000
Viscosity (μ)	2×10^{-3} Pa·s	Fr	1
Thermal conductivity (κ)	100 W/(m·K)	Pe	2500
Specific heat (c_p)	1000 J/(kg·K)	Br	2×10^{-6}
Coefficient of thermal expansion (β)	2×10^{-5} 1/K	Pr	0.02
Surface tension (γ)	1 N/m	We	125
Diameter (d)	0.1 m	Gr	3125000
Velocity (V)	1.0 m/s		
ΔT	10 K		

characteristic parameters are listed at the left side, several dimensionless numbers have been calculated for the flow of molten liquid through a narrow pipe. The values are approximately those of a typical shot sleeve problem.

In this case, where the Reynolds number is particularly high, the inertial forces will dominate the momentum equation. This means that any minor change to the viscosity will have little effect upon the flow profile except through the action of boundary layers [57]. The viscosity could change by several orders of magnitude when liquid metal solidifies.

The *Froude number* represents the ratio between inertial and gravitational forces. In this case, where the Froude number is unity then the inertial and gravitational forces balance. This would suggest that small changes in the density would have some effect upon the flow profile.

The *Weber number* represents the ratio between the inertial and surface tension forces. In this case, where the Weber number is relatively high, the effect of surface tension can be neglected.

The *Peclet number* represents the ratio between the heat transport by convection and the heat transport by conduction. In this case, the Peclet number is high and heat transfer is dominated by convection. This means that a minor change to thermal conductivity has little effect upon the temperature profile, and thus, it is reasonably safe to assume that the thermal conductivity is constant, even when it is not.

The *Brinkman number* is a measure of the importance of viscous heating relative to the heat flow resulting from conduction. In this case, where the Brinkman number is very low it is safe to assume that the effect of viscous heating is negligible.

The *Prandtl number* describes the relative strength of the diffusion of momentum to that of heat. In contrast with the Reynolds number and the Froude number, the Prandtl number is entirely a property of the fluid (and not of the flow). In this case, where the Prandtl number is low, then diffusion of momentum is small.

The *Grashof number* expresses the ratio of buoyancy forces to viscous forces. In

this case, where the Grashof number is very big and is of similar magnitude of the inertia forces, the buoyancy forces which are caused by the density variation should be taken into consideration, i.e., the density should not be assumed constant.

Dimensionless analysis can also be used to make comparisons between independent systems. For example, if two systems have the same Froude and Reynolds number, then both systems are described by identical dimensionless momentum equation. If in addition, the two systems have the same initial and boundary conditions, then the two systems are mathematically identical. Such systems are said to be *dynamically similar*. This situation arises between water and molten metal, which means that water can be used as a *dynamic analogue* to predict the flow characteristics of molten metal. Since it has been found that the flow of water through a pipe is turbulent when the Reynolds number exceeds 2200, and that the majority of casting systems have a Reynolds number that exceeds this value, then it can be concluded, that for the majority of casting systems including the fluid in shot sleeve the flow of molten metal will be turbulent[†]. The Navier-Stokes equations can be averaged over a short time to form a set of time-averaged equations. These equations contain turbulent momentum flux and stress tensors that are non-Newtonian in behavior. Although this behavior can be modeled, it is beyond the scope of the present work. We are

[†]Unfortunately, water does not have the same Brinkman number as molten metal, because if it did, it could be used as a thermal analogue to model solidification. Then, there would be less demand for computer modeling!

primarily concerned with the effects of turbulence, rather than the turbulence itself.

1.6 Turbulence Models

It is observed experimentally that flows above a certain Reynolds number are turbulent. The literature on modeling turbulent flows is enormous. The most commonly used turbulence models seem to be [38]

- algebraic eddy viscosity models (zero equation models)
- $k - \epsilon$ models (two equations models)
- Reynolds stress models

The Reynolds stress models are not introduced here because they are still controversial and because it appears that they may be easier to implement in a compressible flow solver directly.

1.6.1 Zero Equation Models

The easiest turbulence models are the algebraic models of Smagorinsky [39] and Baldwin-Lomax [41]. Most zero equation models consist of the Navier-Stokes equations with a non-constant viscosity (eddy viscosity) μ_T which is a given function of

position x and velocity v . In his subgrid scaled model Smagorinsky suggested

$$\mu_T = \mu + ch^2 |\nabla v + \nabla v^T| \quad (1.4)$$

where μ is the molecular viscosity, c is a numerical constant and $h(x)$ is the average mesh size around x .

The Navier-Stokes equations with the eddy viscosity may develop boundary layers near the walls. An attempt can be made to remove them from the computational domain by replacing the no-slip condition by slip conditions of the type

$$\mathbf{v} \cdot \mathbf{n} = 0 \quad (1.5)$$

$$\mu_T \frac{\partial \mathbf{v}}{\partial \mathbf{n}} \cdot \mathbf{n}_t + \alpha \mathbf{v} \cdot \mathbf{n}_t = \beta \quad (1.6)$$

where $\mathbf{n}$ is the outward normal of the wall, $\mathbf{n}_t$ is the tangent, and α, β may be a non-linear function of $\mathbf{v} \cdot \mathbf{n}_t$ and even $\nabla \mathbf{v}$. Parés [40] has shown that such boundary conditions lead to a well posed problem for the Navier-Stokes equations provided some conditions on the growth of α and β are satisfied.

1.6.2 The $k - \epsilon$ Model

Another commonly used turbulence model is the $k - \epsilon$ model developed by Launder and Spalding in 1972 [42] inspired by Harlow and Nakayama [43]. Let k be the turbulent kinetic energy and ϵ the turbulent rate of dissipated energy. So if v' denotes

the time oscillations of v :

$$k = \frac{1}{2} \langle |v'|^2 \rangle \quad (1.7)$$

$$\epsilon = \frac{\nu}{2} \langle |\nabla v' + \nabla v'^T|^2 \rangle \quad (1.8)$$

In the model it is assumed that the small time oscillations of v , p are equivalent to an eddy viscosity:

$$\mu_T = c_\mu \frac{k^2}{\epsilon} \quad (1.9)$$

and that, away from the walls $k - \epsilon$ are governed by:

$$k_{,t} + v \nabla k - \frac{c_\mu k^2}{2 \epsilon} |\nabla v + \nabla v^T|^2 - \nabla \cdot (c_\mu \frac{k^2}{\epsilon} \nabla k) + \epsilon = 0 \quad (1.10)$$

$$\epsilon_{,t} + v \nabla \epsilon - \frac{c_1 k}{2} |\nabla v + \nabla v^T|^2 - \nabla \cdot (c_\epsilon \frac{k^2}{\epsilon} \nabla \epsilon) + c_2 \frac{\epsilon^2}{k} = 0 \quad (1.11)$$

with $c_\mu = 0.09$, $c_1 = 0.1296$, $c_2 = 1.92$, $c_\epsilon = 0.07$.

Natural boundary conditions could be

$$k, \epsilon \text{ given at } t = 0; \quad k|_\Gamma = k_\Gamma = 0, \quad \epsilon|_\Gamma = \epsilon_\Gamma \quad (1.12)$$

however ϵ_Γ is not known so the model is not well posed near the solid walls. A coupling with a one equation model near the walls can be done. Alternatively an attempt is usually made to remove the low Reynolds regions from the computational domain by applying some wall laws.

At this stage of the research, it was considered premature to model the effective viscosity with complex turbulence models. Only the simplest eddy viscosity model

will be used for turbulence modeling and more sophisticated turbulence modeling is left for future work.

1.7 Numerical Analysis of Heat Transfer

The major challenge to modeling the heat transfer of molten metal has been the phase change or solidification. Transformation from liquid to solid can result in the formation of crystals, as in most metals (crystallization), or the creation of an amorphous state (glass formation). In the case of crystallization, latent heat is evolved at the solid/liquid interface. It is this heat source, together with an often highly complicated interface morphology, which makes it difficult to solve the conservation equations.

Solidification modeling is usually conducted in two scales: microscopic and macroscopic. Most efforts in the field of solidification modeling have used macroscopic modeling, i.e., towards a search for analytical or numerical solutions of the conservation equations in the presence of a phase change, which is also the interest of this research[§]. If one omits analytical solutions, whose use is restricted to simple situations, the numerical techniques which have been used in solidification modeling are quite diverse and include the finite difference method (FDM), the finite element method (FEM),

[§]For those who are interested in the microscopic modeling, see the book by Kurz and Fisher [44], and the review by Rappaz [45].

the boundary element method (BEM), the direct finite difference method (DFDM), the control volume element method (VEM), and many others, which are usually derived from one of the main techniques mentioned here. Although each method has its pros and cons, the finite element method is very popular and is chosen for this research.

In order to deal with heat flow problems in solidification, one can use two basic approaches: front-tracking method (two-domain method) and averaging method (one-domain method), which are schematically illustrated in Fig. 1.4.

Figure 1.4: Schematic representation of two different situations encountered in heat flow modeling of solidification: (a) front-tracking or 2-domain method; (b) 1-domain method. (From [45])

In front-tracking methods, the overall volume within which the conservation of energy is to be solved is sub-divided into 2 domains (liquid and solid) with a solid/liquid interface as shown in Fig. 1.4(a). Accordingly, conservation equations are applied

separately to each domain, plus some continuity equations for the solid/liquid interface. These so-called front-tracking methods, which are quite complicated, are primarily used for the solidification of pure metals or for calculations of isolated cell or dendrite shapes. In averaging methods the solid and liquid phases are considered to be a single domain, with average quantities defined at each node of the mesh as shown in Fig. 1.4(b). Since front-tracking methods are very difficult to apply to general problems of solidification, especially when dealing with alloys which have a mushy zone[¶], one-domain methods are commonly used.

In one-domain methods the heat equation for the total domain which includes the liquid, solid and mushy regions (if they exist) can be written as

$$\nabla \cdot [\kappa \nabla T(\mathbf{X}, t)] + \dot{Q} = c_p \dot{T}(\mathbf{X}, t) \quad (1.13)$$

where κ is the thermal conductivity, c_p is the specific heat per unit volume, and $\dot{Q}$ is the latent heat release which is associated with the phase transformation, and can be written as

$$\dot{Q} = L_h \dot{f}_s(\mathbf{X}, t) \quad (1.14)$$

where L_h is the latent heat, and $\dot{f}_s$ is the rate of formation of fraction of solid at a given *point*, or, to be more precise, within a volume element which is large with respect

[¶]If the liquid-solid interface is not of zero thickness in the mesh, then the liquid-solid interface has finite thickness in the mesh and the phase fraction varies through the thickness. Such a thick liquid-solid interface is called a mushy zone.

to the microstructure and small compared to the temperature inhomogeneities. In the macroscopic modeling of solidification, one neglects any nucleation or growth undercooling and, therefore, f_s is only a function of temperature and $\dot{f}_s = \frac{df_s}{dT} \frac{dT}{dt}$. By inserting Eq. (1.14) into Eq. (1.13), one gets

$$\nabla \cdot [\kappa \nabla T(\mathbf{X}, t)] = c_p \dot{T}(\mathbf{X}, t) - L_h \dot{f}_s(\mathbf{X}, t) = (c_p - L_h \frac{df_s}{dT}) \dot{T}(\mathbf{X}, t) \quad (1.15)$$

The right hand side of Eq. (1.15) can be rewritten according to two different numerical techniques – the *effective specific heat method* and the *enthalpy method*. The effective specific heat method [46, 47, 48] defines the effective specific heat, $c_p^e(T)$, as

$$c_p^e(T) = (c_p - L_h \frac{df_s}{dT}) \quad (1.16)$$

and thus, one has

$$\nabla \cdot [\kappa \nabla T(\mathbf{X}, t)] = c_p^e \dot{T}(\mathbf{X}, t) \quad (1.17)$$

In the enthalpy method [49, 51, 50], the enthalpy H is defined as

$$H(T) = \int_0^T c_p(\theta) d\theta + L_h(1 - f_s(T)) \quad (1.18)$$

and is introduced into Eq. (1.15) to give

$$\nabla \cdot [\kappa \nabla T(H(\mathbf{X}, t))] = \dot{H}[T(\mathbf{X}, t)] \quad (1.19)$$

The effective specific heat method is very popular and has been widely used primarily because the effective specific heat per unit volume can be readily introduced

into standard commercial codes as a tabulated thermophysical property. However, because the $T-f_s$ or $T-H$ curve exhibits discontinuities or strong variations when close to the liquidus or to the eutectic temperature, numerical methods which are based on an effective specific heat have some difficulty in ensuring energy conservation.

On the other hand, the enthalpy method is more difficult to implement in existing codes but it has several advantages. First, energy conservation is ensured. Second, the $H-T$ curve has no singularity, and third, any solidification path is characterized by a strictly decreasing enthalpy; even during recalescence.

For heat flow of molten metal with convection or advection a transport term ($\mathbf{v}(\mathbf{X}, t) \nabla H(\mathbf{X}, t)$) has to be added to Eq. (1.15). Because the Lagrangian formulation is chosen for the numerical simulation, the advection term does not appear.

1.8 Layout of Thesis

This introduction is the first chapter of six. It outlines the aims, objectives and scope of this thesis. The literature review has been conducted to describe the current state of the relevant work. Its aim is to highlight problems and areas of weakness that would suggest promising avenues of research. The nature of the problem is examined by the analysis of the dimensionless parameters. These provide a framework for remaining chapters.

Chapter 2 introduces the governing equations underlining the problem, the finite

element method for spatial discretization and Simo's version of the Newmark algorithm for time integration. Chapter 3 attempts to verify the computer modeling by performing a number of simulations which exhibit well known features of fluid flow and heat transfer. Chapter 4 demonstrates the effects of some parameters on the critical slow shot velocity by numerical experiments, the wave profiles found during these experiments, and the fluid flow and thermal analysis of the slow shot. Chapter 5 discusses the results and recommendations for future work. Chapter 6 presents the conclusions of the research.

Chapter 2

Governing Equations

The equations governing the flow of a fluid and associated heat transfer are based on the conservation of mass, momentum, and energy together with constitutive equations.

2.1 Conservation Equations: Continuous Case in Strong Form

The equations for the conservation of mass, momentum and energy can be written in the following form for an Eulerian or spatial domain.

$$\rho_{,t} + \nabla \cdot (\rho \mathbf{v}) = 0$$

$$\rho [\mathbf{v}_{,t} + \mathbf{v} \cdot \nabla \mathbf{v}] - \nabla \cdot \boldsymbol{\sigma} + \mathbf{b} = 0$$

$$\rho [h_{,t} + \mathbf{v} \cdot \nabla h] + \nabla \cdot \mathbf{q} - p \nabla \cdot \mathbf{v} + Q = 0 \quad (2.1)$$

where ρ is the density field, $\nabla \cdot$ is the divergence operator, σ is the Cauchy stress tensor that satisfies $\sigma \cdot \mathbf{n} = \tau_t$ where $\mathbf{n}$ is the outward normal and τ_t is the traction vector, $\mathbf{b}$ is the body force, h is the specific enthalpy field, $\mathbf{q} = -\kappa_t \nabla T^*$ is the thermal flux field with thermal conductivity tensor κ_t and gradient of the absolute temperature ∇T , p is the pressure and Q is the heat source density or production of heat per unit volume.

The equations for the conservation of mass, momentum and energy can be written in the following form for a Lagrangian or material domain.

$$\begin{aligned} \dot{\rho} + \rho \nabla \cdot \mathbf{v} &= 0 \\ \rho \dot{\mathbf{v}} - \nabla \cdot \sigma + \mathbf{b} &= 0 \\ \rho \dot{h} + \nabla \cdot \mathbf{q} - p \nabla \cdot \mathbf{v} + Q &= 0 \end{aligned} \quad (2.2)$$

where the super-posed dot denotes the substantial or material derivative $\dot{\phi} = \phi_{,t} + \mathbf{v} \cdot \nabla \phi$. For an isotropic Newtonian fluid, the Cauchy stress is

$$\sigma = 2\mu\epsilon - p\mathbf{I} \quad (2.3)$$

where μ is the dynamic shear viscosity, and with

$$\epsilon_{ij} = \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right)$$

*The fluid obeys Fourier's law of heat conduction.

2.2 Conservation Equations: Continuous Case in Weak Form

To solve the weak form of the conservation equations, the following function spaces are defined. The trial function space $\mathcal{V}$ and test function space $\mathcal{V}_0$ for the displacement, velocity and acceleration are

$$\begin{aligned}\mathcal{V} &= \{\mathbf{u} \in [H^1(\Omega)]^3 \mid \mathbf{u}|_{\partial\Omega_D} = \mathbf{u}_D\} \\ \mathcal{V}_0 &= \{\mathbf{u} \in [H^1(\Omega)]^3 \mid \mathbf{u}|_{\partial\Omega_D} = \mathbf{0}\}\end{aligned}\tag{2.4}$$

where $\mathbf{u}|_{\partial\Omega_D} = \mathbf{u}_D$ is the Dirichlet boundary conditions. The trial and test function spaces for the temperature are

$$\begin{aligned}\mathcal{T} &= \{T \in [H^1(\Omega)] \mid T|_{\partial\Omega_D} = T_D\} \\ \mathcal{T}_0 &= \{T \in [H^1(\Omega)] \mid T|_{\partial\Omega_D} = 0\}\end{aligned}\tag{2.5}$$

where $T|_{\partial\Omega_D} = T_D$ is the Dirichlet boundary condition for temperature. The trial and test function spaces for the pressure are

$$\begin{aligned}\mathcal{P} &= \{p \in [L^2(\Omega)] \mid p|_{\partial\Omega_D} = p_D\} \\ \mathcal{P}_0 &= \{p \in [L^2(\Omega)] \mid p|_{\partial\Omega_D} = 0\}\end{aligned}\tag{2.6}$$

where $p|_{\partial\Omega_D} = p_D$ is the Dirichlet boundary condition for pressure field. The space $H^1(\Omega)$ denotes the Sobolev space that is defined by

$$H^1(\Omega) = \{\mathbf{u} \mid \mathbf{u} \in L^2(\Omega), \nabla \mathbf{u} \in L^2(\Omega)\}\tag{2.7}$$

where the space $L^2(\Omega)$ is defined by

$$L^2(\Omega) = \{\mathbf{u} \mid \int_{\Omega} |\mathbf{u}|^2 d\Omega < \infty\} \quad (2.8)$$

With these function spaces defined, the weak form of the conservation of momentum equation in Lagrangian form can be stated

$$a(\rho \dot{\mathbf{v}}, \mathbf{u}) + b(\sigma, \nabla \mathbf{u}) + c(\mathbf{b}, \mathbf{u}) - \langle \sigma \cdot \mathbf{n}, \mathbf{u} \rangle = 0 \quad (2.9)$$

where the above bilinear and linear forms are defined as follows:

$$\begin{aligned} a(\rho \dot{\mathbf{v}}, \mathbf{u}) &= \int_{\Omega} \rho \mathbf{u} \dot{\mathbf{v}} d\Omega \\ b(\sigma, \nabla \mathbf{u}) &= \int_{\Omega} \sigma : \nabla \mathbf{u} d\Omega \\ c(\mathbf{b}, \mathbf{u}) &= \int_{\Omega} \mathbf{b} \cdot \mathbf{u} d\Omega \\ \langle \sigma \cdot \mathbf{n}, \mathbf{u} \rangle &= \int_{\partial\Omega} \sigma \cdot \mathbf{n} \mathbf{u} d\partial\Omega \end{aligned} \quad (2.10)$$

The weak form of the conservation of mass equation in Lagrangian form can be stated as

$$a(\dot{\rho}, u) + b(\rho \nabla \cdot \mathbf{v}, u) = 0 \quad (2.11)$$

where the above bilinear and linear forms are defined as follows:

$$\begin{aligned} a(\dot{\rho}, u) &= \int_{\Omega} \dot{\rho} u d\Omega \\ b(\rho \nabla \cdot \mathbf{v}, u) &= \int_{\Omega} \rho \nabla \cdot \mathbf{v} u d\Omega \end{aligned} \quad (2.12)$$

The weak form of the conservation of energy equation in Lagrangian form can be stated

$$a(\rho \dot{h}, u) + b(q, \nabla u) - c(p \nabla \cdot \mathbf{v}, u) + d(Q, u) + \langle \mathbf{q} \cdot \mathbf{n}, u \rangle = 0 \quad (2.13)$$

where the above bilinear and linear forms are defined as follows:

$$\begin{aligned} a(\rho \dot{h}, u) &= \int_{\Omega} \rho \dot{h} u \, d\Omega \\ b(q, \nabla u) &= \int_{\Omega} \nabla u^T \cdot q \, d\Omega \\ c(p \nabla \cdot \mathbf{v}, u) &= \int_{\Omega} p \nabla \cdot \mathbf{v} u \, d\Omega \\ d(Q, u) &= \int_{\Omega} Q u \, d\Omega \\ \langle \mathbf{q} \cdot \mathbf{n}, u \rangle &= \int_{\partial\Omega} \mathbf{q} \cdot \mathbf{n} u \, d\partial\Omega \end{aligned} \quad (2.14)$$

in which the term $c(p \nabla \cdot \mathbf{v}, u)$ is the reversible heating due to compression, which is negligible in this case.

2.3 Finite Element Equations

Finite element analysis begins by discretizing the spatial domain into a set of elements called a mesh. A finite element mesh partitions the domain into a finite number of convex polyhedra such that every face of a polyhedron is either the intersection of two polyhedra or is the intersection of the polyhedron with the boundary of the domain.

The intersection of any two polyhedra is either the face of a polyhedron or is the empty set. In this thesis, the polyhedra are either bricks, triangular prisms or tetrahedra. An exception to the above rules occurs when the face of a brick is shared by the faces of two tetrahedra. Such a face is called non-conforming and can violate continuity conditions. Associated with each element is a type, a set of nodes, a topology and a set of basis functions. Each element has a reference element, e.g., for brick elements the reference element is usually the cube $((-1 \leq r \leq 1), (-1 \leq s \leq 1), (-1 \leq t \leq 1))$ parameterized by coordinates (r, s, t) . We denote the vector of basis functions for an element as $\mathbf{R}(r, s, t) = \{\varphi_1(r, s, t), \dots, \varphi_{n_n}(r, s, t)\}$ where n_n is usually the number of nodes in the element. The set of elements in the mesh together with the element basis functions define the finite dimensional function spaces for the various fields defined on the mesh. These fields include the following examples.

$$\begin{aligned}
\mathbf{d}(\mathbf{x}(r, s, t)) &= (\mathbf{R}(r, s, t) \bar{\mathbf{d}})^T \\
\mathbf{v}(\mathbf{x}(r, s, t)) &= (\mathbf{R}(r, s, t) \bar{\mathbf{v}})^T \\
\mathbf{a}(\mathbf{x}(r, s, t)) &= (\mathbf{R}(r, s, t) \bar{\mathbf{a}})^T \\
T(\mathbf{x}(r, s, t)) &= \mathbf{R}(r, s, t) \bar{T} \\
p(\mathbf{x}(r, s, t)) &= \mathbf{R}(r, s, t) \bar{p}
\end{aligned} \tag{2.15}$$

the over-bar denotes a $n_n \times \text{dim}$ matrix for vector fields of dimension dim (usually $\text{dim} = 3$) and a n_n dimensional column vector of nodal values for scalar fields.

The isoparametric map from the reference element to the physical element is

$$\mathbf{x}(r, s, t) = (\mathbf{R}(r, s, t) \bar{\mathbf{x}})^T \quad (2.16)$$

where the nodal values $\bar{\mathbf{x}}$ are the spatial coordinates of the nodes, $\mathbf{R}(r, s, t)$ is a row vector of element basis functions.

The Jacobian J maps differentials in (r, s, t) to differentials in (x, y, z) . The inverse of the transpose of the Jacobian J^{-T} maps partial derivatives $(R_{,r}, R_{,s}, R_{,t})^T$ with respect to (r, s, t) to partial derivatives $\nabla R = (R_{,x}, R_{,y}, R_{,z})^T$ with respect to (x, y, z) , i.e.,

$$\nabla R = J^{-T}(R_{,r}, R_{,s}, R_{,t})^T \quad (2.17)$$

Let us also define the following divergence operator in the discretized form as

$$\nabla \cdot \mathbf{R}(r, s, t) = (R_{,x}, R_{,y}, R_{,z}) \quad (2.18)$$

With this background, the FEM operators for the conservation of mass, momentum, and energy equation can be defined. The symbol $\Pi_{e_i=1}^{n_e}$ denotes the operator that assembles element matrices and vectors into global matrices and vectors, n_e is the total number of elements in the domain.

2.4 FEM Discretization of Navier-Stokes Equations

The global matrices for the momentum equation are computed as follows:

- The mass matrix $\mathbf{M} = \Pi_{e_i=1}^{n_e} \int_{\Omega_{e_i}} R^T \rho R d\Omega$. This is one block of the three blocks of the block diagonal mass matrix. If the global matrix is the mass matrix, then each block could be solved separately provided Dirichlet boundary conditions are handled properly for each block. Also the right hand side (RHS) or residual must be computed correctly for each block. This matrix is symmetric positive-definite and only the zero vector is in the null space of this operator.
- The diffusion matrix $\mathbf{C} = \Pi_{e_i=1}^{n_e} \int_{\Omega_{e_i}} \mathbf{B}^T \mathbf{D}_{\text{vis}} \mathbf{B} d\Omega$. This matrix diffuses the momentum, in which the $\mathbf{B}$ matrix and $\mathbf{D}_{\text{vis}}$ are defined as follows:

$$\mathbf{B} = \begin{bmatrix} R_x & 0 & 0 \\ 0 & R_y & 0 \\ 0 & 0 & R_z \\ R_y & R_x & 0 \\ 0 & R_z & R_y \\ R_z & 0 & R_x \end{bmatrix}$$

$$\mathbf{D}_{\text{vis}} = \mu \begin{bmatrix} a0 & a1 & a1 & 0 & 0 & 0 \\ a1 & a0 & a1 & 0 & 0 & 0 \\ a1 & a1 & a0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1. & 0 & 0 \\ 0 & 0 & 0 & 0 & 1. & 0 \\ 0 & 0 & 0 & 0 & 0 & 1. \end{bmatrix}$$

where $a0 = 4/3$ and $a1 = -2/3$ and μ is the dynamic shear viscosity.

The action of viscosity $\mathbf{D}_{\text{vis}}$ is similar to the action of thermal conductivity tensor in the heat equation. This matrix penalizes the deviatoric strain rate and is symmetric positive-semidefinite. A velocity field with zero deviatoric strain rate is in the null space of this operator.

- The divergence matrix is $\mathbf{K}_{\text{div}} = \Pi_{e_i=1}^{n_e} \int_{\Omega_{e_i}} \kappa_b (\nabla \cdot \mathbf{R})^T (\nabla \cdot \mathbf{R}) d\Omega$. The bulk modulus κ_b times the volumetric strain rate is the pressure rate. This matrix would penalize the pressure rate and is symmetric positive-semidefinite. This penalizes the divergence of the velocity and more strongly enforces the divergence free condition if that is desired. Numerical algorithms often use a fictitious value of the bulk modulus if the value of the real bulk modulus would cause ill-conditioning. If the velocity increment and the initial velocity are divergence free, then the nodal velocity vector is in the null space of this matrix.

- The external nodal load $\mathbf{F}^{\text{ext}}$ includes body forces and contributions from Neumann boundary conditions and velocity Dirichlet boundary conditions, in which the body forces are $\mathbf{F}^{\text{b}} = \Pi_{e_i=1}^{n_e} \int_{\Omega_{e_i}} \mathbf{R}_3^T \rho \mathbf{g} d\Omega$, where $\mathbf{R}_3$ is

$$\mathbf{R}_3 = \begin{bmatrix} R & 0 & 0 \\ 0 & R & 0 \\ 0 & 0 & R \end{bmatrix}$$

The contribution from the Neumann tractions is

$$\mathbf{F}^{\text{t}} = \Pi_{e_i=1}^{n_e} \int_{\Gamma_{e_i}} f_x R_f, f_y R_f, f_z R_f) d\Gamma$$

where R_f is the vector of basis functions for a face element, f_x , f_y and f_z are the x , y , and z components of the Neumann tractions.

- The internal force is $\mathbf{F}^{\text{int}}$. For inviscid fluids, the stress is the hydrostatic stress and is equal to pressure times the identity matrix;

$$\mathbf{F}^{\text{int}} = \Pi_{e_i=1}^{n_e} \int_{\Omega_{e_i}} \nabla R^T p d\Omega.$$

If the stress is not hydrostatic, then the more general form is required, that is,

$$\mathbf{F}^{\text{int}} = \Pi_{e_i=1}^{n_e} \int_{\Omega_{e_i}} \mathbf{B}^T \sigma d\Omega.$$

2.4.1 Newmark Methods

In a Lagrangian framework, the Newmark algorithm is commonly used to solve the momentum equation when inertial forces are not neglected. The semidiscrete equation

of motion is written as [54]

$$\mathbf{M}\ddot{\mathbf{d}} + \mathbf{C}\dot{\mathbf{d}} + \mathbf{K}\mathbf{d} = \mathbf{F} \quad (2.19)$$

The initial-value problem for Eq. (2.19) consists of finding a displacement, $\mathbf{d} = \mathbf{d}(t)$, satisfying Eq. (2.19), given initial data:

$$\begin{aligned} \mathbf{d}(0) &= \mathbf{d}_0 \\ \dot{\mathbf{d}}(0) &= \mathbf{v}_0 \end{aligned} \quad (2.20)$$

and boundary conditions.

Equations (2.19) and (2.20) are solved by the classical Newmark family of algorithms, which consists of the following equations:

$$\begin{aligned} \mathbf{M}\mathbf{a}_{n+1} &= \mathbf{F}_{n+1}^{\text{ext}} - \mathbf{F}^{\text{int}}(\tau_{n+1}, \mathbf{d}_{n+1}) \\ \mathbf{v}_{n+1} &= \mathbf{v}_n + \Delta t[(1 - \gamma)\mathbf{a}_n + \gamma\mathbf{a}_{n+1}] \\ \mathbf{d}_{n+1} &= \mathbf{d}_n + \Delta t\mathbf{v}_n + \Delta t^2[(\frac{1}{2} - \beta)\mathbf{a}_n + \beta\mathbf{a}_{n+1}] \end{aligned} \quad (2.21)$$

where $\mathbf{d}_n$, $\mathbf{v}_n$, and $\mathbf{a}_n$ are the approximations of $\mathbf{d}(t_n)$, $\dot{\mathbf{d}}(t_n)$, and $\ddot{\mathbf{d}}(t_n)$, respectively, and τ is the Kirchhoff stress defined as $\tau(\mathbf{x}, t) = \det(F(\mathbf{X}, t)) \sigma(\mathbf{x}, t)$, in which F is the deformation gradient.

This time stepping algorithm by the classic Newmark family is enforced at t_{n+1} and two noteworthy properties of this class of schemes are [55]:

1. The only member of the classical Newmark family that preserves exactly conservation of total angular momentum (for equilibrated loading) is the *explicit*

central difference method obtained for $\beta = 0$ and $\gamma = 1/2$.

2. The Newmark-*trapezoidal* rule, corresponding to the values $\gamma = 1/2$ and $\beta = 1/4$, does not inherit the conservation property of total angular momentum.

Simo's Version of Newmark Algorithm

Consider the algorithm defined by the semidiscrete momentum equation (2.19) enforced in conservation form at $t_{n+\alpha}$ along with the standard Newmark formulae [55]; i.e.,

$$\begin{aligned} \mathbf{M}(\mathbf{v}_{n+1} - \mathbf{v}_n) &= \mathbf{F}_{n+\alpha}^{\text{ext}} - \mathbf{F}^{\text{int}}(\tau_{n+\alpha}, \mathbf{d}_{n+\alpha}) \\ \mathbf{d}_{n+1} &= \mathbf{d}_n + \Delta t[(1 - \frac{\beta}{\gamma})\mathbf{v}_n + \frac{\beta}{\gamma}\mathbf{v}_{n+1}] + \Delta t^2(\frac{1}{2} - \frac{\beta}{\gamma})\mathbf{a}_n \\ \mathbf{a}_{n+1} &= \frac{1}{\gamma\Delta t}(\mathbf{v}_{n+1} - \mathbf{v}_n) + (1 - \frac{1}{\gamma})\mathbf{a}_n \end{aligned} \quad (2.22)$$

where $\mathbf{d}_{n+\alpha} := \alpha\mathbf{d}_{n+1} + (1 - \alpha)\mathbf{d}_n$ and $\mathbf{F}_{n+\alpha}^{\text{ext}} := \alpha\mathbf{F}_{n+1}^{\text{ext}} + (1 - \alpha)\mathbf{F}_n^{\text{ext}}$, and $\tau_{n+\alpha}$ denotes the Kirchhoff stress evaluated at the generalized mid-point configuration. This algorithm has the following noteworthy properties.

1. Choosing values for parameters of $\alpha = 1/2$, $\beta = 1/2$ and $\gamma = 1$, the algorithm is acceleration independent, exact momentum preserving, mid-point rule in conservative form. This is true only at the mid-point. There are no spurious modes.

2. The implicit mid-point rule does define an A-contractive algorithm in the non-linear regime, i.e., unconditionally stable.

Simo solves for velocity $\mathbf{v} \equiv \dot{\mathbf{d}}$ at the mid-point. Then uses an update procedure to compute displacement $\mathbf{d}$ and acceleration $\ddot{\mathbf{d}}$ at the end of the time step. Simo approximates the acceleration at the mid-point of the time interval by

$$\mathbf{a} = \ddot{\mathbf{d}} = \frac{[\dot{\mathbf{d}}_{n+1} - \dot{\mathbf{d}}_n]}{\Delta t} \equiv \frac{[\mathbf{v}_{n+1} - \mathbf{v}_n]}{\Delta t} \equiv \frac{D\mathbf{v}}{\Delta t} \quad (2.23)$$

The exact solution for the velocity increment from time t_n to time t_{n+1} can be written as the sum of a trial solution and the error in the solution, i.e., as

$$\begin{aligned} D\dot{\mathbf{d}}_{n+1}^{\text{exact}} &= D\dot{\mathbf{d}}_{n+1}^{\text{trial}} + d\dot{\mathbf{d}}_{n+1}^{\text{error}} \\ D\mathbf{v}^{\text{exact}} &= D\mathbf{v}^{\text{trial}} + d\mathbf{v}^{\text{error}} \end{aligned} \quad (2.24)$$

Each Newton-Raphson iteration solves the following equations for the correction $d\mathbf{v}$ to the increment of the velocity $D\mathbf{v}$.

$$\begin{aligned} \mathbf{K}_{\text{eff}}[d\mathbf{v}] &= \Delta t \mathbf{F}_{n+\alpha}^{\text{ext}} - \Delta t \mathbf{F}^{\text{int}}(\tau_{n+\alpha}, \mathbf{v}_n + \alpha D\mathbf{v}) - \mathbf{M}[D\mathbf{v}] \\ D\mathbf{v} &:= D\mathbf{v} + d\mathbf{v} \end{aligned} \quad (2.25)$$

where $\mathbf{K}_{\text{eff}}$ is the effective stiffness matrix. We would write this in our notation as:

$$\begin{aligned} \mathbf{K}_{\text{eff}} &= \mathbf{M}_{n+\alpha} + \alpha_1 \Delta t \mathbf{C}_{n+\alpha} + \alpha_2 \Delta t^2 \mathbf{K}_{n+\alpha} \\ \mathbf{F}_{n+\alpha}^{\text{ext}} &= (1 - \alpha) \mathbf{F}_n^{\text{ext}} + \alpha \mathbf{F}_{n+1}^{\text{ext}} \end{aligned}$$

$$\begin{aligned}
\mathbf{RHS} &= \Delta t \mathbf{F}_{n+\alpha}^{\text{ext}} - \Delta t \mathbf{F}^{\text{int}}(\tau_{n+\alpha}, \mathbf{v}_n + \alpha D\mathbf{v}) - \mathbf{M}[D\mathbf{v}] \\
\mathbf{K}_{\text{eff}} d\mathbf{v} &= \mathbf{RHS} \\
D\mathbf{v} &:= D\mathbf{v} + d\mathbf{v}
\end{aligned} \tag{2.26}$$

where $\alpha_1 = \frac{1}{2}$ and $\alpha_2 = \frac{1}{4}$.

After convergence is reached for this time step, the displacement and acceleration are updated according to Eq. (2.22). Simo recommends the values $\alpha = 0.5$, $\gamma = 1.0$ and $\beta/\gamma = 0.5$. This simplifies the update formulae to

$$\begin{aligned}
\mathbf{d}_{n+1} &= \mathbf{d}_n + \frac{\Delta t}{2} [\mathbf{v}_n + \mathbf{v}_{n+1}] = \mathbf{d}_n + \Delta t \mathbf{v}_n + \frac{\Delta t}{2} [D\mathbf{v}] \\
\mathbf{a}_{n+1} &= \frac{\mathbf{v}_{n+1} - \mathbf{v}_n}{\Delta t}
\end{aligned} \tag{2.27}$$

More important, it guarantees an A-contractive algorithm in the non-linear regime, i.e., unconditionally stable.

2.4.2 Quasi-Statically Admissible Pressure Field

Given an open domain in $\Omega \in \mathbb{R}^3$ with sufficiently smooth boundaries, velocity and acceleration fields that satisfy the conservation of mass, a sufficiently smooth viscous stress field and a body force field $\rho \mathbf{g}$, then a quasi-statically admissible pressure field on the domain can be defined as a C^0 pressure field such that ∇p satisfies the following discrete weak formulation

$$\Pi_{e_i=1}^{n_e} \left[\int_{\Omega_{e_i}} [\mathbf{R}_3^T (\rho \mathbf{a} + \mathbf{B}^T \sigma_{\text{vis}} + \nabla p + \rho \mathbf{g})] d\Omega + \left(\int_{\Gamma_{e_i}} \mathbf{R}_3^T \tau d\Gamma \right) \right] = 0$$

$$\text{i.e.,} \quad a(\rho \dot{\mathbf{v}}, \mathbf{u}) + b(\nabla \mathbf{v}, \nabla \mathbf{u}) + c(\nabla p, \mathbf{u}) + d(\mathbf{b}, \mathbf{u}) + \langle \boldsymbol{\tau}, \mathbf{u} \rangle = 0 \quad (2.28)$$

The integrand in the above equation is a vector force field. Taking the divergence of the integral, one obtains the following pressure Poisson equation.

$$\begin{aligned} \left[\Pi_{e_i=1}^{n_e} \int_{\Omega_{e_i}} \nabla \mathbf{R}^T \nabla \mathbf{R} d\Omega \right] \bar{p} &= \Pi_{e_i=1}^{n_e} \left[\int_{\Omega_{e_i}} \left[\nabla \mathbf{R}^T (\rho \mathbf{a} + \mathbf{B}^T \sigma_{\text{vis}} + \rho \mathbf{g}) \right] d\Omega \right] \\ \text{i.e.,} \quad \mathbf{K}_{\text{QSP}} \bar{p} &= \mathbf{R}_{\text{QSP}} \end{aligned} \quad (2.29)$$

Since the only unknown in the above equation is the pressure field, the nodal pressure field can be computed by solving the above equation together with any Dirichlet pressure boundary conditions for the nodal pressures $\bar{p}$.

This is an instance of a pressure Poisson equation which is similar to the pressure Poisson equation used by Yabe [58] and Zienkiewicz [69]. However, it differs from them in that the velocity is assumed to satisfy the conservation of mass equation. In solving this equation, the viscous stress is evaluated at volume Gauss points, then projected to nodes, averaged at nodes and interpolated back to volume Gauss points. Note that this pressure field is such that the nodal forces in the momentum equation balance exactly. These nodal forces are projections from Gauss point force densities to nodal forces. It is important to note that it is the discrete forces on nodes that are in equilibrium and that the forces on individual elements are not in equilibrium. Thus the momentum equation is a balance of nodal forces in the sense

of d’Alambert’s principle (i.e., simply include the element inertia forces as part of the body force.). If the equation was satisfied pointwise, it would be statically admissible. Since it is only satisfied in the weak sense, it is said to be quasi-statically admissible. The velocity, displacement and acceleration are nodal fields evaluated at times t_n and t_{n+1} . The velocity and displacement fields were required to satisfy Dirichlet boundary conditions. The viscous stress and pressure are nodal fields evaluated at times $t_{n-1/2}$ and $t_{n+1/2}$. The body force $\rho \mathbf{g}$ is given data. Note that the only kinematic data specified in this equation is the acceleration which is used to evaluate the inertial force.

2.4.3 Incompressible Flow

Gresho [59] distinguishes between an incompressible flow and an incompressible material. An incompressible material has infinite bulk modulus, infinite speed of sound and the density at each point is constant in time. Even though incompressible flow is often defined to be a flow such that $\nabla \cdot \mathbf{v} = 0$, the more general definition of incompressible flow does not require $\nabla \cdot \mathbf{v} = 0$. Nor does it require the density to be constant in time or in space [56]. Incompressible flow does require that;

1. Changes in density due to changes in pressure can be neglected.
2. The speed of the fluid is small relative to the speed of sound.

3. The ‘height’ length is small relative to the ‘height length scale’ $p/(\rho g)$ which is 8.4 km for the earth’s atmosphere.

In this thesis, the flow of liquid metal will be considered incompressible in this more general sense.

The difficulty in computing the numerical solution to problems of incompressible flow is due to the stiffness or ill-conditioning caused by the high bulk modulus or volumetric stiffness relative to the elastic or viscous shear stiffness. More precisely when the bulk modulus is less than 1×10^4 N/m² and the dynamic viscosity of liquid aluminum is 1×10^{-3} Pa·s, then the iterative solvers such as the Incomplete Cholesky Conjugate Gradient solver (ICCG) and Symmetrized Successive Over Relaxation Conjugate Gradient solver (SSORCG) [60] converge rapidly, say in 50 iterations for a 1000-element mesh of 8-node bricks. If the bulk modulus is increased by a factor of ten, the iterative solvers no longer converge in 5000 iterations. This is caused by the increase in the condition number. The standard strategy for dealing with slightly compressible or incompressible materials is to use a mixed method in which the unknown fields are the displacement or velocity and the pressure. Then solve a 2×2 system in which the incompressibility is enforced by a Lagrange multiplier.

The element must be chosen carefully to define appropriate discrete velocity and pressure spaces. If an element satisfies the Ladyzhenskaya, Brezzi, Babuska (LBB)

condition, then the solution to the 2×2 system will have no spurious pressure modes. Elements that satisfy the LBB condition are discussed in detail in [66]. In this thesis, the 8-node brick element Q1-P0 will be used with piecewise discontinuous constant pressure. In spite of the fact that this element does not satisfy the LBB condition and can have a spurious checkerboard pressure mode which will be filtered, this element is popular.

In this thesis, the quasi-static pressure solver filters any spurious modes of the Q1-P0 element that might appear. An interesting element that does satisfy the LBB condition is the non-conforming Rannacher-Turek 6-node brick [67, 68]. It is the FEM analogue of the popular Marker and Cell (MAC) FDM method.

Having chosen a mixed element, one must choose an algorithm to solve the 2×2 system of equations. The most popular methods are either some form of Uzawa's algorithm (see Appendix A) or a pressure projection method. In this thesis, a version of the pressure projection method is used.

2.4.4 Pressure Projection Method

The pressure projection method solves a pressure Poisson equation for pressure and then uses this pressure field to compute velocity correction that is intended to make the velocity field satisfy the incompressibility constraint. There are several strategies for implementing the pressure projection method [59]. First the discrete pressure

Poisson equation can be formed in at least two ways. One way forms the continuous pressure Poisson equation and then discretizes it. This leads to a standard discrete Laplacian operator. An alternative is to form the pressure Poisson equation as the Schur complement of the 2×2 system of equations. In this case the Jacobian is computed by a triple product of matrices. For C^0 pressure spaces, the matrices must be global. For elements with discontinuous pressure function space, the triple product of matrices can be performed at the element level and the pressure unknowns can be condensed out at the element level (see Appendix B). From the literature, this appears to be the most popular method. In this thesis, the global pressure Poisson equation will be formed as the Schur complement of the discrete 2×2 global system of equations. Given a velocity field $\mathbf{v}'$, the projected velocity field $\mathbf{v}_p$ is computed as

$$\begin{aligned} \mathbf{B}_{\text{div}} \mathbf{M}_{\text{lumped}}^{-1} \mathbf{B}_{\text{div}}^T \hat{p} &= -\frac{1}{\Delta t} \nabla \cdot \mathbf{v}' \\ \mathbf{v}_p &= \mathbf{v}' - \frac{\Delta t}{\rho} \nabla \hat{p} \end{aligned} \quad (2.30)$$

where $\mathbf{B}_{\text{div}}$ is computed as $\Pi_{e_i=1}^{n_e} (\int_{\Omega_{e_i}} (\nabla \cdot \mathbf{R}) d\Omega)$, $\mathbf{M}_{\text{lumped}}$ is the global lumped mass matrix, and $\nabla \cdot \mathbf{v}'$ is the divergence of velocity evaluated at the element centroids.

2.5 FEM Discretization of Energy Equation

For a Lagrangian formulation the mesh velocity with respect to the material velocity is zero and the advective term disappears. The Galerkin formulation of the energy

equation for a time integration scheme defined by a parameter $0 \leq \alpha \leq 1$ for space discretized by an FEM mesh Ω^h and a time interval $[t_1, t_3]$ with initial conditions $T_1 \equiv T(t_1)$ and solution $(T_3 \equiv T(t_3), DH_{\text{Latent}})$ is

$$\begin{aligned} \rho c_p G(T_3) + \Delta t \alpha K_{\text{diff}}(T_3) &= \rho c_p G(T_1) - G(DH_{\text{Latent}}) - \Delta t K_{\text{diff}}(1 - \alpha) T_1 \\ &\quad - \Delta t \alpha S_3 - \Delta t(1 - \alpha) S_1 \end{aligned} \quad (2.31)$$

where DH_{Latent} is the nodal thermal load vector due to the increment in latent heat from time t_1 to t_3 , $S_1 \equiv S(t_1)$ and $S_3 \equiv S(t_3)$ are the nodal thermal load vectors due to external loads at time t_1 and t_3 , the time step length is $\Delta t \equiv t_3 - t_1$. The global Gram matrix is formed by assembling the element Gram matrices, i.e., $G = \Pi_{e_i=1}^{n_e} (\int_{\Omega_{e_i}} \mathbf{R}^T \mathbf{R} d\Omega)$. The global diffusion matrix K_{diff} is formed by assembling the element diffusion matrices, i.e., $K_{\text{diff}} = \Pi_{e_i=1}^{n_e} (\int_{\Omega_{e_i}} \nabla \mathbf{R}^T \kappa_t \nabla \mathbf{R} d\Omega)$ where κ_t is the thermal conductivity tensor.

Contributions to the stiffness operator from convection boundary conditions and interface contact conductance are discussed below.

If the equation is formulated in terms of T_1 and H_1 and $DT + dT = T_3 - T_1$ and $DH + dH = H_3 - H_1$ where DT and DH are the current trial solutions of the temperature and specific enthalpy increments and dT and dH are the corrections or the errors, then the equation for the Galerkin formulation becomes

$$c_p G(DT + dT) + G(DH_{\text{Latent}} + dH_{\text{Latent}})$$

$$\begin{aligned}
& +\Delta t \alpha K_{\text{diff}} (T_1 + DT + dT) + \Delta t (1 - \alpha) K_{\text{diff}} (T_1) \\
& +\Delta t \alpha S_3 + \Delta t (1 - \alpha) S_1 = 0
\end{aligned} \tag{2.32}$$

The only unknown terms are dT and dH_{Latent} . Combining $G c_p DT + G DH_{\text{Latent}} = G DH$ and moving all known terms to the right hand side which is then the residual, we have

$$\begin{aligned}
c_p G (dT) + \Delta t \alpha K_{\text{diff}} (dT) + G (dH_{\text{Latent}}) &= -G DH \\
& -K_{\text{diff}} \Delta t (\alpha DT + T_1) \\
& -\Delta t \alpha S_3 - \Delta t (1 - \alpha) S_1
\end{aligned} \tag{2.33}$$

The convection boundary condition, $q = k(T - T_{\text{amb}})$ is decomposed into two terms, in which k denotes the convection coefficient and T_{amb} is the ambient temperature. The contribution from the convection boundary condition to the stiffness matrix on the left side is

$$\int_{\Gamma_{f_i}} k \mathbf{R}^T \mathbf{R} d\Gamma \tag{2.34}$$

The contribution from the convection boundary condition to the residual or RHS vector is

$$\left(\int_{\Gamma_{f_i}} \mathbf{R}^T \mathbf{R} d\Gamma \right) \left[k(\bar{T}_{\text{amb}} - \bar{T}_1 - \alpha \bar{DT}) \right] \tag{2.35}$$

There is a contribution from contact stiffness to the global stiffness on the left hand side $\Delta t \alpha K_{\text{cont}}$ and to the residual or RHS $[K_{\text{cont}}] [\Delta t \alpha (\bar{DT} + \bar{T}_1)]$ that can be included at the element level. Here K_{cont} is the contact stiffness.

The global system of equations is solved using an ICCG solver with Newton-Raphson iterations. Usually, the value of α is set to 1.0 which is a backward Euler scheme for integration in time.

For each Newton-Raphson iteration we assume that $dH_{\text{Latent}} = 0$, and solve for a trial correction $d\tilde{T}$. This $d\tilde{T}$ implies a correction to the specific enthalpy $c_p d\tilde{T} = dH$ that can be decomposed into $dH = c_p dT + dH_{\text{Latent}}$ by a pointwise solidification solver. With these values of dT and dH , convergence is tested and if convergence has not been achieved, another Newton-Raphson iteration is performed.

2.5.1 Interface Contact Conditions

Heat transfer through contact surfaces, i.e., interfaces formed by the contact of two different materials, e.g., the interface between the casting and mould in die casting, depends upon a number of parameters such as the thermal properties of gases/fluids in the interface, surface roughness characteristics, applied mechanical load, microhardness characteristics of solids, etc. In a die-casting process, the progress of solidification depends on the heat transfer coefficient at the mould-cast interface, which can vary significantly during cooling process. A gap at the mould-cast interface surface can form and increase which can change the heat transfer pattern. Most analytical and experimental studies are reported in terms of thermal contact conductance which is the reciprocal of the thermal contact resistance.

Following Dhatt *et al.* [61], we write the interface conductance as the sum of contributions from several heat transfer mechanisms

$$\kappa_{\text{IF}} = \kappa_{\text{asp}} + \kappa_{\text{gas}} + \kappa_{\text{rad}} + \kappa_{\text{conv}} \quad (2.36)$$

Asperity Conductance

Because two surfaces in contact do not fit together perfectly, most of the energy transferred flows through a limited number of actual contact spots or asperities. The interface contact conductance due to asperities

$$\kappa_{\text{asp}} = \beta p^\alpha \quad (2.37)$$

is a function of the normal traction $p = \sigma \cdot \mathbf{n}$ in which σ is the Cauchy stress tensor and $\mathbf{n}$ the outward normal vector, and α and β that are functions of temperature and interface properties. If there is a gap, the interface surfaces do not touch, then the normal traction is zero and $\kappa_{\text{asp}} = 0$.

Radiation Conductance

The thermal interface conductance due to radiation is

$$\kappa_{\text{rad}} = k_B f_\epsilon \left(T_{\text{cast}}^2 + T_{\text{mold}}^2 \right) (T_{\text{cast}} + T_{\text{mold}}) \quad (2.38)$$

where k_B is the Boltzmann's constant (1.38×10^{-23} J/K) and f_ϵ is the relative emissivity function of the gap surfaces.

Gas Conductance

The thermal interface conductance κ_{gas} is due to the interface conductance of the gas in the gap. In aluminum castings, the gas is likely to be hydrogen. In steel castings, the gas is likely to be a mixture of CO and CO₂. If the gap width is W and the molecular thermal conductivity of the gas is k_{gas} , then

$$\kappa_{\text{gas}} = \frac{k_{\text{gas}}}{W} \quad (2.39)$$

In foundry problems, the thickness of the air gap is very small, so the air conduction term is relatively important, and the interface conductance due to convection cells in the gas is usually negligible. So, if there is a gap, the thermal interface conductance is taken to be [62]:

$$\kappa_{\text{IF}} = \kappa_{\text{gas}} + \kappa_{\text{rad}} = \frac{k_{\text{gas}}}{W} + k_B f_{\epsilon} (T_{\text{cast}}^2 + T_{\text{mold}}^2) (T_{\text{cast}} + T_{\text{mold}}) \quad (2.40)$$

Chapter 3

Verification of Software

The software was designed and developed using object-oriented programming (OOP), which allows future extensions to be added easily. To solve the fluid flow problem with free surface three main classes were developed; the Pressure Solver, the Incompressible Flow Solver and the Divergence Free Projection (DFP) Solver. The Incompressible Flow Solver solves a 2×2 system which includes the Pressure Solver and DFP Solver. Given the initial condition of displacement, velocity and acceleration, the quasi-statically admissible pressure field is first solved by the Pressure Solver. Then the Navier-Stokes equations (the conservation of mass and the conservation of momentum in Eq. 2.2) are solved for the velocity field by the Incompressible Flow Solver. To avoid locking [52] a finite bulk modulus is used which means the Navier-Stokes equations are solved with some compressibility. Finally, the DFP Solver corrects the

velocity field to make it divergence free.

To do the thermal analysis the Energy Solver was developed. The non-linearity due to solidification is dealt with by implementing a method similar to the enthalpy method and by performing Newton-Raphson iterations so that the energy is conserved.

3.1 Pressure Solver

The Pressure Solver solves the pressure field at time $t_{n+1/2}$ for a given state such as velocity, acceleration, temperature and gravity.

3.1.1 Hydrostatic Test

If the fluid is at rest, $\mathbf{a} = \mathbf{0}$ and $\mathbf{v} = \mathbf{0}$. Based on Equations (2.2) and (2.3) the pressure field reduces to

$$\nabla p = \rho \mathbf{g} \quad (3.1)$$

This is a hydrostatic pressure distribution and is correct for all fluids at rest, regardless of the viscosity, because the viscous term vanishes identically.

If $\mathbf{g} = (0, 0, -g)^T$, where $g = 9.8 \text{ m/s}^2$, the pressure is only a function of the z coordinate and can be expressed as

$$p(z) = p_0 + \rho g(z_0 - z) \quad (3.2)$$

where p_0 is the pressure at the free surface and z_0 is the coordinate of the free surface in the z direction.

The test was set up as follows:

- The mesh is $10 \times 1 \times 10$ with element size = 0.01 m.
- The pressure at free surface is set to 0.
- $\mathbf{v} = \mathbf{0}$ and $\mathbf{a} = \mathbf{0}$.
- $\mathbf{g} = (0, 0, -9.8)^T$.
- $\rho = 1000 \text{ kg/m}^3$.

The exact solution was obtained by the Pressure Solver.

3.1.2 Couette and Poiseuille Flow

Consider a two-dimensional incompressible plane ($\partial/\partial z = 0$) with viscous flow between parallel plates a distance $2h$ apart, as shown in Fig. 3.1. Fig. 3.1a is *Couette flow* due to a moving boundary: a linear velocity profile with no-slip at each wall, gravity effects neglected. The momentum equation (in Eqs. (2.2)) reduces to $\nabla \cdot \sigma = 0$. According to Eq. (2.3) the pressure distribution reduces to $\nabla p = \mathbf{0}$, i.e., p is constant.

The test was set up as follows:

- The mesh is $10 \times 1 \times 10$ with element size = 0.01 m.

Figure 3.1: Velocity profile: (a) Couette flow; (b) Poiseuille flow. (From [53])

- $\mathbf{v} = (10y, 0, 0)^T$ and $\mathbf{a} = \mathbf{0}$.

- $\mathbf{g} = \mathbf{0}$.

The pressure computed by the Pressure Solver is zero which is the exact solution.

Fig. 3.1b is Poiseuille flow due to a parabolic velocity profile with no-slip at each wall. Gravity effects are neglected. The pressure is only a function of x and can be expressed as

$$\frac{dp}{dx} = -\frac{2v_{\max}\mu}{h^2} \quad (3.3)$$

The test was set up as follows:

- The fluid has size of $0.1 \times \text{element size} \times 0.1$ m and was meshed with element size = 10, 5, 2.5, 1 and 0.5 mm, respectively.
- The outlet surface is set to zero pressure.

- $\mathbf{v} = (400y(0.1 - y), 0, 0)$ and $\mathbf{a} = \mathbf{0}$.
- $\mathbf{g} = \mathbf{0}$.
- $\mu = 1.0 \text{ kg}/(\text{m}\cdot\text{s})$.

The distribution of the pressure field for the mesh with element size of 1 mm is shown in Fig. 3.2. The pressure is constant along the y -axis and decreases linearly along the x -axis according to the curve which was sampled along the center line. The exact solution for dp/dx is -800.0 Pa and the numerical solution is -793.8 Pa.

Figure 3.2: Pressure distribution in Poiseuille flow.

Tests were conducted with meshes of different element sizes. The error of the pressure gradient decreases linearly as the mesh becomes finer as shown in Fig. 3.3. This suggests that the error comes from the 8-node brick element which has linear basis functions to approximate the parabolic velocity field. Mathematically, the discretization error in a variable is of the order $O(h^{p+1-m})$ [69], where h is an element size, p is the order of Taylor expansion, and m is the m th derivatives appearing in the norm of the error. For an 8-node brick element, the error in velocity is of the order $O(h^2)$. The error in pressure gradient is of the order $O(h)$ because the pressure gradient is equal to the first derivative of velocity. Thus, the error in pressure gradient is a linear function of element size.

The 20-node brick mesh was used to verify that the element type is the cause of the error. The pressure gradient is linear and the solution is exact for a 20-node brick mesh with element size of 5 mm*.

3.2 DFP Solver

The DFP Solver projects the velocity field to a divergence-free velocity field. A 1D test was setup as follows:

- The 8-node brick mesh is $10 \times 1 \times 1$ with element size = 0.01 m.

*The exact solution is expected even for a single 20-node brick element mesh in this case.

Figure 3.3: The error of the pressure gradient versus mesh size in Poiseuille flow.

- $v_y = 0$, $v_z = 0$ for all nodes, and $v_x = 1$ at $x = 0$ which are the Dirichlet boundary condition.
- $v_x = 0$ at $x > 0$.

The DFP Solver solves the velocity field and the velocity is $(1, 0, 0)^T$ for each node which is the exact solution and divergence free.

Several approaches were tried that did not work well. These include the following:

1. Yabe's pressure Poisson equation is a discretization of the continuous or infinite dimensional pressure Poisson equation [58]. A solver which was formulated according to Yabe was tested using the same test problem above and the velocity

field was not divergence-free. It appears that the incompressible constraint is enforced at Gauss points in some weak sense.

2. A pressure Poisson solver on a MAC grid (staggered mesh) is similar to that of a structured mesh with 6-node brick elements. It does satisfy the divergence constraint accurately for the MAC grid. However, after mapping the velocity field from the MAC grid to the 8-node brick mesh the velocity field on the 8-node brick mesh no longer satisfied the divergence constraint.
3. A potential solver somewhat similar to that of Khayat [17] was developed and tested but it was abandoned because a method to deal with the singularity at the intersection of the free surface and the plunger face could not be devised.

3.3 Incompressible Flow Solver

The Incompressible Flow Solver involves time steps in which the discrete momentum equation is solved by Simo's Newmark method. Multiple time steps are conducted to check the correctness for the following tests.

3.3.1 Free Fall Test

An object in the air will fall under the influence of gravity. If the drag or friction is neglected, the velocity and displacement are given by

$$v(t) = v_0 + gt \quad (3.4)$$

$$d(t) = v_0 t + \frac{1}{2}gt^2 \quad (3.5)$$

The test was set up as follows:

- The mesh is $10 \times 10 \times 10$ with element size = 0.01 m.
- $\mathbf{v}(t) = \mathbf{0}$ and $\mathbf{a}(t) = \mathbf{0}$ at $t = 0$.
- All the boundary faces are free surface with $p = 0$.
- $\mathbf{g} = (0, 0, -9.8)^T$.

The Incompressible Flow Solver gives the exact results.

3.3.2 Steady-State Poiseuille Flow

If the fluid is at rest at $t = 0$ s and a parabolic velocity (as shown Fig. 3.1b) is applied at the entrance, the velocity field will evolve toward a steady-state Poiseuille flow at sufficiently long times provided the velocity is sufficiently slow, i.e., a low enough Reynolds number. The test was set up as follows:

- The mesh is $10 \times 1 \times 10$ with element size = 0.01 m.
- $\mathbf{v}(t) = \mathbf{0}$ and $\mathbf{a}(t) = \mathbf{0}$ at $t = 0$.
- $p = 0$ at $x = 0.1$, i.e., the outlet surface.
- $v_x = 400y(0.1 - y)$ at $x = 0$ and no-slip boundary condition is applied.
- $\mathbf{g} = (0, 0, 0)^T$.
- $\mu = 1.0 \text{ kg}/(\text{m}\cdot\text{s})$, and $\rho = 1000 \text{ kg}/\text{m}^3$.

After 200 time steps (time step size = 1 ms), the velocity and pressure fields are very close to the fully-developed Poiseuille flow as shown in Fig. 3.4.

Figure 3.4: Steady-state Poiseuille flow: (a) the pressure field at $t = 0.2 \text{ s}$; (b) the velocity field at $t = 0.2 \text{ s}$.

The velocity field is developed quite well except at the outlet where there are non-zero y components of velocity as shown in Fig. 3.5. This probably comes from an inconsistency between the *kinematically admissible stress* (KAS) which is used in the Incompressible Flow Solver and *quasi-statically admissible stress* (SAS) which is used in the Pressure Solver.

Figure 3.5: The directions of velocity field in steady-state Poiseuille flow.

3.3.3 Dam Break

A common test problem for programs which simulate free boundary value problems is that of the ‘dam break’ [23], in which a vertical wall confining a fluid to one side of a basin is suddenly removed, thereby allowing the fluid to spread out. The test was set up as follows:

- The liquid column has size of $0.1143 \times \text{element size} \times 0.1143$ m (0.1143 m = 4.5 in) and was meshed with element size = 3, 2 and 1 mm, respectively.
- The pressure at free surface is set to 0.
- $\mathbf{v}(t) = \mathbf{0}$ and $\mathbf{a}(t) = \mathbf{0}$ at $t = 0$.
- A slip boundary condition is applied, i.e., the fluid can slide without friction[†].
- $\mathbf{g} = (0, 0, -9.8)^T$.
- $\mu = 1.0$ kg/(m·s), and $\rho = 1000$ kg/m³.
- Time step size is 0.003 s.

The pressure and velocity fields at $t = 0.16$ s for the mesh with element size of 3 mm are shown in Fig. 3.6.

[†]A test with no-slip boundary condition was conducted for comparison.

Figure 3.6: Collapse of a fluid column under the influence of gravity: (a) the pressure at $t = 0.16$ s; (b) the velocity at $t = 0.16$ s.

It was noticed that the mesh density has little effect on the profile of the liquid. This is an important result because it confirms the relative independence of the simulation from the mesh density. If this were not so, then our confidence in any solution would be clouded by our choice of mesh.

Large deformation of elements occurred in the Dam-Break test. The distortion metric developed by Oddy *et al.* [64] was used to measure the element distortion. The method first normalizes the Jacobian matrix to remove the effect of element size by

$$J'_{ij} = \frac{J_{ij}}{|J|^{1/n}}$$

where n is the number of dimensions. Then the distortion metric can be expressed as

$$DM = E_{ij}E_{ij} - \frac{1}{n}(E_{kk})^2 \quad (3.6)$$

where DM is the distortion metric and $E_{ij} = J'_{ki}J'_{kj}$.

The remeshing was conducted when DM exceeded some criteria. Fig. 3.7a illustrates the badly distorted mesh before remeshing. After remeshing, the mesh is quite uniform and the geometry is preserved quite well as shown in Fig. 3.7b. The volume change is used to measure the performance of the remeshing and is about -0.05% (volume loss). Data was mapped from the old mesh to the new mesh, and the problem continued to be solved.

The tests were also repeated by running with different time step sizes to investigate the effect of the Courant number on the conservation of mass or volume loss. It was

Figure 3.7: The meshes: (a) before remeshing; (b) after remeshing.

observed that the maximum velocity at the surge front reaches 2.2 m/s. Based on this maximum velocity, the Courant number (Co) is computed as

$$Co = \frac{v\Delta t}{l} = \frac{v_{\max}\Delta t}{2l} \quad (3.7)$$

where Δt is the time step size and l is the average element size which is 3 mm. As the Courant number decreases, the volume loss of the fluid decreases as shown in Table 3.1.

[‡]Number of time steps are different but the simulation times are the same for the three tests.

Table 3.1: The effect of Courant number on the volume loss

Time step size (ms)	1.0	2.0	3.0
Number of time steps [†]	450	300	150
Courant number	0.37	0.73	1.1
Volume loss (%)	2.0	4.1	5.6

The positions of the surge front for the tests with slip boundary condition and with no-slip boundary condition[§] were obtained and compared with the experimental data by Martin and Moyce [71] as shown in Fig. 3.8. The computed results with a slip boundary condition match experimental results much better than those with a no-slip boundary condition, which implies that the boundary layer is relatively thin and no-slip boundary condition is too strong a constraint for the mesh used. In addition, the number of remeshing steps for the no-slip and slip test are 75 and 3, respectively, i.e., the no-slip test required 25 times more remeshing steps than the slip test.

The discrepancy between the numerical and experimental results at later times comes from the assumption of a slip boundary condition and possibly ignoring surface tension. The effects of friction and surface tension become more significant at later times when the slip velocity becomes faster and the front becomes thinner.

[§]The fluid can not slide at the bottom boundary.

Figure 3.8: Distance traveled by the surge front during the collapse of a fluid column.

In reality, no-slip boundary conditions should be enforced on each wetted surface when solving the Navier-Stokes equations. If one solved the potential flow equations, then slip boundary conditions should be imposed on wetted surfaces. If no-slip boundary conditions are enforced on wetted surfaces, then the free surface and wetted surface intersect on a curve that is a manifold of co-dimension 2 for the 3-D shot sleeve wave problem. This curve moves and associated with the movement of this

curve one requires a constitutive equation. Furthermore, the constitutive equation must deal with both a static and dynamic motion of the curve, i.e., the difficult stick-slip problem [63]. Experimental data for such constitutive equations is difficult to obtain. The length scales are expected to be small relative to the length scales in the shot sleeve wave problem. In this thesis, the detailed physics of the contact curve is neglected.

Imposing no-slip boundary conditions with conforming contact elements would significantly increase the cost and complexity of meshing as can be seen from the Dam-Break test. This could be manageable using methods from domain decomposition or by using a space-time formulation that allows a mesh velocity different from the material velocity. In any case, in this thesis it was decided that the benefits of enforcing a no-slip boundary condition on wetted surfaces were not outweighed by their cost and complexity.

3.4 Energy Solver

The Energy Solver was initially developed for the thermal analysis of a die casting. A test suite was established to test the correctness of the Energy Solver. The test suite includes the tests such as diffusion test, calorimetric heating and cooling test, convection boundary test, flux boundary test and contact test. Both static and transient tests and transient tests with solidification are included. The test suite is

run routinely and all the tests are routinely conducted and passed. In this research the convection boundary and transient solidification are relevant. See the paper by Goldak *et al.* [65] for details.

Chapter 4

Thermal and Fluid Flow Analysis in a Shot Sleeve

In this chapter the domain, initial and boundary conditions for the fluid flow analysis of a slow shot in a die casting shot sleeve are addressed first. The analyses for a 2-D shot sleeve, i.e., the vertical symmetry plane of the cylindrical shot sleeve and a 3D cylindrical shot sleeve are presented. Numerical experiments were conducted to determine the critical slow shot velocity. Several patterns of wave formation for different plunger profiles were obtained. Later, the flow and heat transfer of molten metal in a shot sleeve were investigated by coupling the Navier-Stokes equations and conservation of energy, and corresponding results will be presented.

Table 4.1: Material properties for liquid Aluminum 380 at 850 K

Density	2760 kg/m ³
Viscosity	0.004 N·s/m ²
Bulk modulus	6.7647×10 ¹⁰ N/m ²
Specific heat	1013 J/(kg·K)
Coefficient of thermal expansion	1.48×10 ⁻⁵ 1/K
Melting temperature	850 K
Thermal conductivity	109 W/(m·K)
Latent heat	9.2015×10 ⁸ J/m ³

4.1 Material Properties

The material chosen for the following tests is Aluminum 380. Its relevant material properties are listed in Table 4.1.

4.1.1 Viscosity

Because of the turbulent nature of the flow during the slow shot the effective viscosity, which is the sum of the molecular and turbulent viscosity, is several orders of magnitude higher than the molecular viscosity [16, 70]. At this stage, it would be impractical to model the effective viscosity. Therefore a constant value of eddy

viscosity is used that is simply two orders of magnitude higher than the real viscosity. The viscosity is constant in the sense that it is not a function of the velocity field. The effects of solidification on the viscosity are still taken into account, i.e., the viscosity is a function of enthalpy which is computed by the Energy Solver.

4.1.2 Bulk Modulus

An effective bulk modulus of 1000 N/m^2 is used in the numerical experiments. This is seven orders of magnitude lower than the real bulk modulus. This is to avoid ill-conditioning that would make the Navier-Stokes equations hard to solve. In the DFP Solver, the real bulk modulus can be used.

4.1.3 Density

As the buoyancy force is relatively large in the analysis, the density variation is taken into account by assuming the density is a function of enthalpy.

4.2 Fluid Flow Domain

Unlike the Eulerian methods of which the domain usually includes the air and liquid, the domain for this research only includes the molten metal which is more natural because the effect of air pressure on the liquid is small during the slow shot. Only

the molten metal domain is meshed.

The RLE Mesher which was developed earlier for the analysis of filling process was used to make the meshes. RLE is an abbreviation for Run Length Encoding – a data compression technique which is used in sending a fax. In this research it has been used in meshing algorithms to store the intersection points of the lines in a Cartesian grid with the surface of a body which is usually defined by an STL (STereo Lithographic) file. The STL file defines a set of triangles that in the ideal case forms a two-manifold of a part such as the casting that partitions space into points inside the part and points outside the part. Each triangle is defined by twelve real numbers; the (x, y, z) coordinates of the three vertices of the triangle and the outward normal of the triangle (n_x, n_y, n_z) . The STL file stores no topology. An example of the mesh made by RLE Mesher is shown in Fig. 4.1, which has approximately 60,000 elements.

For simple geometries such as a half cylinder the Primitive Mesher, which is basically the parametric mesher, is preferred since it represents the geometry accurately with fewer elements. The initial liquid grid in the cylindrical shot sleeve meshed by the Primitive Mesher is presented in Fig. 4.2 and it contains about 10,000 8-node brick elements.

Figure 4.1: An example of the mesh created by the RLE Mesher.

4.3 Boundary Conditions for Fluid Flow Analysis

The concept of a boundary constraint $\mathcal{C}(t)$ is required to apply the boundary condition for the fluid flow analysis.

An impermeable boundary is a constraint such that any object inside the boundary cannot penetrate. In this research two special kinds of boundary constraints are considered, a rectangle block $\mathcal{C}_r(t)$ for a 2-D shot sleeve and a cylinder $\mathcal{C}_c(t)$ constraint for a 3-D shot sleeve. An STL file can be a constraint in the filling process of die casting although it is only used for making a mesh in the current research as mentioned

Figure 4.2: An example of the mesh created by the Primitive Mesher.

in the previous section.

At any instant of time the configuration of the fluid is assumed to occupy a region in space $\Omega(t)$ bounded by $\Gamma(t)$. The boundary $\Gamma(t)$ is composed of a liquid-air free surface, $\Gamma_f(t)$, and liquid-solid interface or boundary $\Gamma_s(t) \subseteq \mathcal{C}(t)$, i.e.,

$$\Gamma(t) = \Gamma_f(t) \cup \Gamma_s(t) \quad (4.1)$$

$$\Gamma_s(t) = \Gamma_{cw}(t) \cup \Gamma_{ew}(t) \cup \Gamma_p(t) \quad (4.2)$$

where $\Gamma_{cw}(t)$ is the cylindrical part of the solid boundary that is wetted, $\Gamma_{ew}(t)$ is

the end part of the solid boundary that is wetted, and $\Gamma_p(t)$ is the wetted surface in contact with the moving plunger.

One fact to be noticed is that $\Gamma_s(t) \cap \Gamma_f(t) \neq \emptyset$, i.e.,

$$\Gamma_s(t) \cap \Gamma_f(t) = \Gamma_{sf}(t) \quad (4.3)$$

$$\Gamma_{ss}(t) \cup \Gamma_{sf}(t) = \Gamma_s(t) \quad (4.4)$$

$$\Gamma_{ff}(t) \cup \Gamma_{sf}(t) = \Gamma_f(t) \quad (4.5)$$

where $\Gamma_{sf}(t)$ is the part which belongs to both free surface and solid boundary, Γ_{ss} is the part which belongs only to the liquid-solid boundary, and Γ_{ff} is the part which belongs only to the liquid-air free surface.

The Dirichlet boundary condition for the Pressure Solver is straightforward and can be expressed as

$$p(\mathbf{x}, t) = p_{\text{air}} \quad \mathbf{x} \subseteq \Gamma_f(t) \quad (4.6)$$

where p_{air} is the air pressure which is set to 0. It is convenient to assume that the plunger moves in the Cartesian x direction and that its center passes through the point $(0, 0, 0)$. Then the Dirichlet boundary conditions for the Incompressible Flow Solver and DFP Solver can be applied as

$$v_x(\mathbf{x}, t) = \begin{cases} v_p(t) & \mathbf{x} \subseteq \Gamma_p(t) \\ 0 & \mathbf{x} \subseteq \Gamma_{ew}(t) \end{cases} \quad (4.7)$$

where v_x is the x component of the velocity, v_p is the plunger velocity, and

$$\mathbf{v}(\mathbf{x}, t) \cdot \mathbf{n} = 0 \quad \mathbf{x} \subseteq \Gamma_{cw}(t) \quad (4.8)$$

where $\mathbf{n}$ is the outward normal of the surface.

It is assumed that the gravity acts in the negative z direction. Then the plane $y = 0$ is a symmetry plane which means the y component of a point including internal points on the plane can be set as Dirichlet degree of freedom (DOF) and its value is 0, i.e.,

$$v_y(\mathbf{x}, t) = 0 \quad \text{at } \mathbf{x}(x, 0, z) \quad (4.9)$$

To implement the boundary condition of Equation (4.8), a local coordinate system is used to apply the Dirichlet DOF, i.e., the rotation matrix (R) for the node is defined to rotate the velocities so that it has normal component and tangential components. Only the normal component is set to Dirichlet DOF and its Dirichlet value is 0. The normal component in the local coordinate system is assigned the z component in solving global equations because the x component is reserved for the plunger axis and outward normal of the end wall and y component is reserved for symmetry. The columns of R for a node are the Cartesian basis vectors $[e_1, e_2, e_3]$ of the local coordinate system. e_1 is chosen to be $(1, 0, 0)^T$ and e_2 is chosen to be the tangential direction of the cylinder which is $(0, z/r, -y/r)^T$, where y and z are the coordinates of the node in y and z directions, and r is the radius of the cylinder. Then e_3 is the cross product of e_1 and e_2 which is equal to $(0, y/r, z/r)^T$.

For each element a constraint matrix C_R is built by assembling R for each node that has a local coordinate system. If a node is not assigned a local coordinate system, then $R \equiv I$ is the identity matrix. The constrained element stiffness matrix is $C_R^T K C_R$ and constrained element vectors are $C_R^T V$.

4.4 Initial Conditions for Fluid Flow Analysis

The initial condition for the fluid flow analysis in slow shot is very simple. The fluid is assumed to be at rest after pouring the metal into the shot sleeve, i.e.,

$$\mathbf{v}(\mathbf{x}, t) = \mathbf{0}; \quad \mathbf{a}(\mathbf{x}, t) = \mathbf{0}; \quad \text{at } t = 0 \quad (4.10)$$

4.5 Critical Slow Shot Velocity

The time-power acceleration law is used and the plunger velocity during the acceleration can be expressed as

$$V(t) = \alpha t^n \quad (4.11)$$

where α is a positive coefficient and n is a non-negative constant. The acceleration $a(t)$ for $n > 0$ is

$$a(t) = \frac{dV}{dt} = \alpha n t^{n-1} \quad (4.12)$$

If $n = 1$, we get the constant acceleration with $a = \alpha$. The plunger profile for the slow shot is shown in Fig. 4.3, i.e., (a) start from zero velocity; (b) constant acceleration to reach some velocity; (c) move with constant velocity. All the tests conducted below followed this parameterization of the plunger profile.

Figure 4.3: Plunger velocity versus time for the slow shot profile.

It has been widely accepted in the literature that there exists a critical slow shot velocity (V_c). According to the literature, the critical slow shot velocity can be defined as the maximum plunger velocity reached during slow shot acceleration such that the molten liquid just barely reaches the ceiling just in front of the plunger without the wave breaking or rolling over.

There are three main parameters that influence the critical slow shot velocity: the

inner diameter of a shot sleeve (D), the acceleration (a) and the initial fraction filled (IFF).

4.5.1 Effects of Inner Diameter of a Shot Sleeve

The effect of inner diameter of a shot sleeve on the critical velocity is presented in Fig. 4.4. The critical velocity increases as the inner diameter increases. The numerical results are compared with the analytical results by Garber and they match quite well.

Figure 4.4: Inner diameter of a shot sleeve versus the critical slow shot velocity. The data was obtained from numerical analyses with a 2-D shot sleeve.

The volume loss is obtained for 210 time steps with a Courant number of 0.37 and is 2.2%. Of this volume loss, the volume loss by remeshing is negligible.

4.5.2 Effects of Acceleration

The effect of acceleration on the critical velocity is shown in Fig. 4.5. The critical velocity decreases as the acceleration increases although the magnitude is relatively small. The acceleration does affect the shape of the wave as shown in Fig. 4.6. The thickness or width of the wave decreases as the acceleration increases. Usually, the wave becomes more stable as the wave thickness increases which suggests a larger velocity range to reach the ceiling of shot sleeve without rolling over. However it has been noticed that the wave could break away if the acceleration is too small, say, less than 1.0 m/s^2 . This phenomenon will be discussed in Section 4.6. Therefore, accelerations of around 2 m/s^2 are recommended for shot sleeve diameters in the range of 50 to 150 mm.

4.5.3 Effects of Initial Fraction Filled

Fig. 4.7 shows the effect of initial fraction filled on the critical velocity. As the initial fraction filled decreases, the critical velocity increases.

A comparison of the numerical and analytical results is also shown in Fig. 4.7. And they match quite well.

It was observed that the wave became less stable as the initial fraction filled decreased toward 0.3. For low fractions filled, the simulated results indicate that the wave could break at the middle of the free surface even before a full height wave can

Figure 4.5: Acceleration versus the critical slow shot velocity. The data was obtained from numerical analyses with a 2-D shot sleeve.

be created.

4.6 Patterns of Wave and Air Entrapment

Generally, three patterns of the wave most often found in the literature are shown in Fig. 1.3. Variations from these three patterns have also been found during the numerical experiments to determine the critical slow shot velocity as shown in Fig. 4.8.

Fig. 4.8a is the case when the plunger velocity is slower than the critical velocity ($V < V_c$). Because of the slow plunger velocity a full height wave is not created in

Figure 4.6: Acceleration versus the shape of the wave. The data was obtained from numerical analyses with a 2-D shot sleeve.

front of the plunger and the wave travels faster than the plunger. When the wave reaches the far end of the shot sleeve, it will be reflected and the reflected wave could fill the runner. This could entrap a large air bubble in front of the plunger.

Fig. 4.8b shows the case when the plunger velocity is approximately equal to the critical velocity, i.e., the velocity is just fast enough to make a full height wave without breaking or rolling. An appropriate acceleration is also important to keep the wave from rolling over by increasing the wave thickness as discussed in Section 4.5.2. This is the wave pattern which entraps no air or the least air.

If the velocity is larger than the critical velocity ($V > V_c$), the wave will reach full height, and curl over from the ceiling or break as shown in Fig. 4.8c. This will

Figure 4.7: Initial fraction filled versus the critical slow shot velocity. The data was obtained from numerical analyses with a 2-D shot sleeve.

entrap air within the molten metal.

The patterns shown above are the three patterns found most often in literature. Fig. 4.8d shows the pattern when the plunger velocity is slightly slower than the critical velocity. Again, the wave is not able to reach the ceiling just in front of the plunger but instead touches the ceiling some distance ahead of the plunger face because the combined efforts of the moving plunger and the reflected wave from the far end of the shot sleeve. This will entrap air similar to that of Fig. 4.8a but a lesser amount. This is the wave pattern which has not been reported in literature.

When the plunger accelerates at a very low rate, i.e., the velocity reaches its maximum at the very end of the plunger travel or slow shot displacement, the slope

Figure 4.8: Patterns of wave formation. The plunger is on the left side. The data was obtained from numerical analyses with a 2-D shot sleeve.

of the wave becomes very flat. In this case the effect of the wave striking the end of the shot sleeve seems to be more significant. The wave tends to crest in the middle of the wave front and entrap air between the plunger and the wave crest as shown in Fig. 4.8e. This phenomenon was mentioned by Tszeng and Chu in their theoretical work [9].

Fig. 4.8f shows the case of low initial fractions filled, e.g., 0.3. In this case the wave front is very unstable even when the plunger velocity is at the critical velocity or less. It breaks in the middle of the wave and entraps air at an early stage of the slow shot. It is very difficult to manage a stable wave front without a trade-off as will be discussed later.

4.7 Wave Analysis in Cylindrical Shot Sleeve

Consider the 3-D transient flow inside a partially filled cylindrical shot sleeve. The motion of the fluid is induced by the movement of a plunger inside the shot sleeve of a die casting machine. The dimensions of the shot sleeve and flow conditions are similar to those encountered in practice. The length of the cylinder is taken as 40 cm with a diameter of 10 cm. The initial mesh which is created by the Primitive Mesher is shown in Fig. 4.2. If at any time the mesh distortion measure exceeds a specified tolerance, then remeshing is done. An example of the mesh that has been remeshed by the RLE Mesher is shown in Fig. 4.1. This mesh contains 8-node brick,

6-node prism and 4-node tetrahedral elements. The plunger movement is simulated by moving the left end of the cylinder. The plunger in this example is assumed to move according to the plunger profile shown in Fig. 4.3. An acceleration due to the gravity of $(0, 0, -9.8)^T$ is applied.

It would be helpful to compute some characteristic times such as acceleration time (t_a) and filling time (t_f). The acceleration time is simply

$$t_a = \frac{v_{\max}}{a} \quad (4.13)$$

where $v_{\max}$ is the maximum plunger velocity and a is the acceleration. The distance traveled (d_a) during the acceleration period is

$$d_a = \frac{1}{2}at_a^2 = \frac{v_{\max}^2}{2a} \quad (4.14)$$

The distance (d_f) traveled by the plunger to fully fill the shot sleeve is

$$d_f = (1 - IFF)L$$

where IFF is the initial fraction filled and L is the shot sleeve length. If $d_f > d_a$, the filling time is

$$t_f = t_a + \frac{d_f - d_a}{v_{\max}} = \frac{(1 - IFF)L}{v_{\max}} + \frac{v_{\max}}{2a} \quad (4.15)$$

The fluid flow analysis is done for the following plunger profile parameters and IFF values shown in Table 4.2.

Table 4.2: The settings for the fluid flow analysis

Setting	$v_{\max}$ (m/s)	a (m/s ²)	IFF	t_a (s)	d_a (m)	t_f (s)
1	0.56	1.5	0.5	0.373	0.1045	0.544
2	0.40	1.5	0.5	0.267	0.0533	0.633
3	0.70	2.0	0.5	0.350	0.1225	0.461
4	0.70	3.3	0.5	0.212	0.0742	0.392
5	0.90	2.0	0.3	0.450	0.2025	0.536

The results of Setting 1 for the full filling process are shown in Fig. 4.9. The cavity is initially filled with a fluid considered to be at rest as shown in Fig. 4.9a. During the acceleration period the fluid continues to rise against the plunger. At $t = 0.264$ s, which is the time when the plunger travels about half the distance of the acceleration process, it is observed that the elevation of the fluid in front of the plunger is highest and flat, and the wave built is very smooth as shown in Fig. 4.9b. At $t = 0.373$ s, the time when the plunger reaches the maximum velocity, the fluid at the plunger is very close to the ceiling of the cylinder as shown in 4.9c. It is observed that the fluid continues to rise because of the momentum built during the acceleration, and comes in contact with the ceiling at $t = 0.397$ s as shown in Fig. 4.9d. The filling near the ceiling part seems to go very fast as shown in Fig. 4.9e and the gap between the wave and ceiling is filled at $t = 0.494$ s as shown in Fig. 4.9f. Fig. 4.9g shows

there is a little bit of roll over at $t = 0.534$ s and the fluid almost completely fills the cylindrical cavity at $t = 0.550$ s as shown in Fig. 4.9h. The total volume loss for 276 time steps and Courant number of 0.38 is 2.8%, of which 0.5% is from the three remeshing steps. The plunger parameters chosen seem to make an ideal filling process for the slow shot. Thus, the maximum velocity of 0.56 m/s seems to be the critical velocity and the wave built by the acceleration is also thick and stable.

If the maximum velocity is smaller than the critical velocity as in setting 2, the full height wave is not achieved and the wave is far from reaching the ceiling when the acceleration process ends as shown in Fig. 4.10a. In this case the wave travels faster than the plunger as shown in Fig. 4.10b. As the wave moves away from the plunger, the height of the wave continues to grow. At a later time, the wave is reflected from the far end of the shot sleeve. This leads to the entrapment of a large volume of air in front of the plunger as shown in Fig. 4.10c.

If the maximum velocity is greater than the critical velocity as in setting 3, it is observed that the full height wave is reached at $t = 0.302$ s even before the acceleration process ends as shown in Fig. 4.11a. As the acceleration continues, the wave tends to roll over as shown in Fig. 4.11b, and shoots ahead at the ceiling of the cylinder as shown in Fig. 4.11c.

If the acceleration is higher still as in setting 4, it is observed that the elevation is higher at the cylindrical part than the middle as shown in Fig. 4.12a. Also the

Figure 4.9: Evolution of flow with time inside a shot sleeve during the slow shot for Setting 1.

wave is relatively thin compared to Fig. 4.9b. The wave tends to roll over and shoots ahead at the ceiling of the cylinder as shown in Fig. 4.12b, which is similar to Fig. 4.11c.

For a slow shot with low initial fraction filled as in setting 5 the fluid front is unstable at an early stage of the filling as shown in Fig. 4.13a and the wave will curl over at both sides of the cylinder (shown in Fig. 4.13b) and trap a large volume of air as shown in Fig. 4.13c.

4.8 Thermal Analysis in Cylindrical Shot Sleeve

The heat transfer between molten metal and shot sleeve or plunger is strictly by contact. There are three difficulties in the computational modeling of heat transfer with conforming contact elements in this analysis. First, the shot sleeve and plunger must be in the domain which would increase the difficulty of the meshing task which is already substantial. Second, even if the shot sleeve and plunger were meshed and included in the domain, it is still not clear how to move the nodes in the shot sleeve and plunger to be compatible with those in molten metal so that the computation in contact elements could be conducted. Third, the initial temperature distribution in the shot sleeve is unknown and is complicated by the fact that the shot sleeve is repeatedly filled and then ejected. A cyclic steady-state temperature field will be reached that is dependent on the thermal analysis of this research. In this case,

it is assumed that the initial temperature in the shot sleeve is constant and the temperature field in the shot sleeve and plunger does not change during the slow shot. With these assumptions, the contact boundary condition can be replaced by a convection boundary condition with the convection coefficient being the contact conductance and the ambient temperature initial shot sleeve temperature.

For each time step a thermal analysis is done after the velocity field is solved and material points are advected by the displacement field computed by the Newmark method. The domain for thermal analysis is the same as the domain for flow analysis. The convection boundary condition is applied for all boundary faces, i.e.,

$$q = k(T - T_{\text{amb}}) \quad \mathbf{x} \in \Gamma(t) \quad (4.16)$$

where T_{amb} is the ambient temperature which is set to 500 K, and k is the convection coefficient of which $k = 5000 \text{ W}/(\text{m}^2 \cdot \text{K})$ if $\mathbf{x} \subseteq \Gamma_p(t)$, $k = 1000 \text{ W}/(\text{m}^2 \cdot \text{K})$ if $\mathbf{x} \subseteq \Gamma_s(t)$ and $k = 10 \text{ W}/(\text{m}^2 \cdot \text{K})$ if $\mathbf{x} \subseteq \Gamma_f(t)$.

The initial temperature of the liquid aluminum is set to 900 K.

The thermal results with the plunger profile with maximum velocity of 0.56 m/s and acceleration of 1.5 m/s^2 , i.e., setting 1, are shown in Fig. 4.14.

Fig. 4.14a shows the initial state of molten liquid. It is observed that the temperature is lower near the plunger face and higher at the free surface, and at $t = 0.287 \text{ s}$ the corner near the plunger face starts to solidify as shown in Fig. 4.14b. At $t = 0.406 \text{ s}$, the whole face near the plunger solidifies as shown in Fig. 4.14c. The solidification

only occurs adjacent to the plunger during the slow shot as shown in Fig. 4.14d. For most of the liquid metal that is likely to enter the runner during the fast shot, the temperature drop is in the range of 0-30 K as shown in Fig. 4.14e.

Figure 4.10: Fluid flow inside a shot sleeve with slower plunger velocity.

Figure 4.11: Fluid flow inside a shot sleeve with faster plunger velocity.

Figure 4.12: Fluid flow inside a shot sleeve with faster plunger velocity and acceleration.

Figure 4.13: Fluid front inside a shot sleeve with low initial fraction filled.

Figure 4.14: Evolution of temperature with time inside a shot sleeve during the slow shot.

Chapter 5

Discussion and Future Work

5.1 Wave Patterns

The critical slow shot velocities attained numerically are compared with the analytical and experimental results and they match quantitatively.

If the plunger travels at the critical velocity with fraction filled near 0.5, air entrapment should be minimal. Behind the wave, the fluid completely fills the cross-section area of the shot sleeve cylinder. In front of the wave, the fluid remains mostly at the initial fill level. Virtually all air is pushed ahead of the wave, out the shot sleeve cylinder, into the runner.

Plunger velocities less than the critical velocity results in an air gap above the surface of the wave. At a later stage, the wave front strikes the ejector die, splashing

upward. Air in the gap will be trapped.

Plunger velocities greater than the critical velocity results in a breaking wave causing violent mixing of air and fluid in front of the wave.

These wave patterns match those observed in the water-analogue experiments [4] qualitatively.

For low initial fill levels, the wave rises, loses vertical velocity, and tumbles forward before it touches the top of the shot sleeve cylinder. A breaking wave is formed, and significant air entrapment results. For the constant acceleration plunger profiles as shown in Fig. 4.3, although the best choice of acceleration may lead to a significant reduction in air entrapment, it may still not be possible to create a stable wave front with this type of profile when very low fractions filled are used. For this range of fraction filled, the simulated results indicate that the wave could break at the middle of the free surface even before a full height wave can be created. Garber also observed the phenomena for low fractions filled. If the plunger acceleration is slowed to avoid instability, the velocity will not reach the critical velocity before the end of the slow shot. One important conclusion from this result is that a shot sleeve with lower initial fraction filled is very sensitive to the choice of plunger profile. It will be difficult to maintain a stable wave front. Therefore, it is recommended that the initial fraction filled should be near 0.5 and should not go below 0.3 since this low fraction filled requires very careful shot control to avoid creating a breaking wave. In this research

all attempts to avoid a breaking wave led to excessively slow shot times and/or partial solidification of metal in the sleeve.

5.2 The Acceleration Law

Minimizing the cycle time will increase the production rate in die casting. This section addresses the overall effects of the acceleration law during the slow shot on the production rate of the die casting process.

In most experimental and analytical studies, the plunger velocity is assumed to increase linearly with the distance traveled, resulting in an acceleration which grows exponentially with time (see Eq. (1.3)). The reason for this choice is that the plunger velocity profiles are typically programmed by specifying the plunger velocity as a function of plunger position. This profile is not discussed here because the sudden decrease of acceleration from maximum to zero has an adverse impact on the fluid flow by common sense, which is probably why there is trapped air in some experimental and analytical results reported [8, 12].

In this research the acceleration is constant in the plunger profile, i.e., $n = 1$ in Equation (4.12). If $n = 0$, the velocity is constant for all time, i.e., instantaneous acceleration to the maximum velocity. In this case minimum filling time is achieved.

The distance traveled during the acceleration (d'_a) is

$$d'_a = \int_0^{t'_a} V(t)dt = \frac{v_{\max} t'_a}{n+1} \quad (5.1)$$

in which t'_a is the acceleration time and $v_{\max} = \alpha t_a^n$ is applied. Assume $d'_a = d_a$ (computed in Eq. (4.14)), i.e., the distance traveled by any acceleration law is equal to the distance traveled by the constant acceleration. Then

$$t'_a = \frac{n+1}{2} \frac{v_{\max}}{a} \quad (5.2)$$

Thus, the time saved is

$$\Delta t = t_a - t'_a = \frac{1-n}{2} \frac{v_{\max}}{a} \quad (5.3)$$

It can be seen from Eq. (5.3) that the filling time can be minimized only if $n < 1$. The maximum time saved is $\Delta t_{\max} = v_{\max}/(2a)$ when $n = 0$, which is half the acceleration time by constant acceleration law.

Let $v_{\max} = 0.56$ m/s and $a = 1.5$ m/s² as in Setting 1 of Table 4.2, the maximum time saved is 0.19 s. A parabolic velocity profile ($n = 0.5$) is more practical for a real die casting machine and in this case Δt is 0.09 s. Compared to the cycle time for a large die casting which is usually in the range of 60 s, the time saved during the slow shot is negligible. The filling time for slow shot is 0.544 s as shown in Table 4.2. So the time saved for the filling of the slow shot is about 17 % which is modest. Now that the temperature drop for liquid metal which will most likely to enter the

die cavity is in the range of 0-30 K, the temperature drop would be expected to be in the range of 0-25 K provided the parabolic velocity profile is applied. The gain in minimizing the filling time avoids very little solidification or cooling of the liquid metal. Therefore it is clear that the reason for optimizing the plunger profile is to minimize trapped air and improve yield and quality of casting and it is not to reduce the casting cycle time to increase the production rate.

If we increase the acceleration for the constant acceleration case, i.e., increase α for Eq. (4.11), the filling time may decrease according to Eq. (4.15) if $v_{\max}$ is assumed unchanged. Actually as the acceleration increases, the critical velocity decreases. In this case, it is not clear that the filling time will be minimized. In addition, an increase in the acceleration could create a thin and unstable wave front and lead to large volume of air entrapment.

5.3 Conservation of Mass

In the numerical experiments a loss of fluid mass (numerical leak) has been noted and measured. The possible reasons for the volume loss are listed below:

1. Errors in the discrete time integration, i.e., the time step size or the Courant number is too large.
2. The discretization in space which is mainly related to the remeshing and mesh

displacement computed from the flow solver.

3. The numerical mass leaks which are related to the enforcement of the constraint such as

- The attribute of a point $\mathbf{x}$ may change during the analysis. For example, $\mathbf{x}(t_1) \subseteq \Gamma_{ff}(t_1)$ can switch to $\mathbf{x}(t_3) \subseteq \Gamma_s(t_3)$, i.e., a pure free surface point can become a boundary constrained point if it moves onto the constraint surface. During a time step a pure free surface point can even move out of the constraint surface. In this case the point will be pulled back to the constraint surface which will cause some numerical leak.
- A breaking wave with itself, i.e., the free surface intersects itself as shown in Fig. 4.8f.
- For cylindrical shot sleeve it is possible that a point of $y < 0$ at t_1 moves to $y > 0$ at t_3 (points around the symmetry plane) or *vice versa*. This is another kind of collision and was dealt with by simply projecting the point onto the symmetry plane, i.e., $y = 0$.
- Usually the tangential components of velocities at the cylindrical part of shot sleeve are not zero and a node can move out of the constraint. A numerical leak happens when it is pulled back onto the cylinder.

Table 5.1 summarizes the volume loss for different tests.

Table 5.1: Volume loss of the fluid

Test	Dam-Break	2-D Shot Sleeve	3-D Shot Sleeve
Average Courant number	0.37	0.37	0.38
Number of time steps	450	210	276
Total volume loss (%)	2.0	2.2	2.8
Volume loss by remeshing (%)	0.0	0.0	0.5
Volume Loss per time step*(%)	0.004	0.010	0.008
Reason(s)	1	1, 3	1, 2, 3

The effect of Courant number on the volume loss can be demonstrated in Table 3.1. As the Courant number decreases, so does the volume loss and it has the largest effect on the conservation of mass. The reason is that the divergence free projection is done at the configuration of t_1 , i.e., using the Euler time integration scheme. The nodes are advected by this div-free velocity field. Then the nodes are checked and corrected if there is any numerical leak described above. If the projection is done at the configuration of t_3 , i.e., using the implicit time integration scheme, the geometric non-linearity from the numerical leaks related to the constraint may lead to a slow convergence. Thus, the Euler integration scheme in the DFP Solver is used, and for this reason a smaller time step size is needed and is usually in the order of 1 ms.

*The volume loss by remeshing is not included.

The numerical leaks related to the constraint also have some effect on the volume loss by comparing the volume losses between the Dam-Break test and 2-D shot sleeve test. The magnitude of the effect is limited and should decrease as the time step size decreases. The overall volume loss in the cylindrical shot sleeve is equivalent to that in the 2-D shot sleeve although the cylindrical shot sleeve has more possibilities to leak.

The remeshing for 3-D cylindrical shot sleeve does show some volume loss of the fluid although the magnitude is modest compared to the effect of the Courant number. The Arbitrary Lagrangian-Eulerian formulation may be implemented so that the distortion in the spatial mesh could be minimized, which would delay the remeshing step and increase the time between remeshing.

5.4 Future Work

The future work can include the improvements and extensions of the current work.

The improvements are listed as follows:

1. Improvement of the remeshing algorithm. There are two approaches to deal with the badly-distorted geometry – Arbitrary Lagrangian-Eulerian (ALE) and a better mesher. Usually ALE supports improving a spatial mesh with fixed topology so that the remeshing could be delayed. Even with ALE a better

mesher is necessary because ALE will ultimately fail to cope with mesh distortion. A mesh with smooth surfaces is of particular importance for the fluid flow analysis with free surfaces.

2. Improving the slip boundary condition. It was noticed that the slip or no-slip boundary condition does affect the fluid flow in the Dam Break test. A wall law similar to Eq. (1.6) from the algebraic eddy viscosity models could accurately approximate the friction force for the slip boundary condition.
3. Implement condensing a 2×2 system for incompressible flow at element level. This is a very popular method which is described in Appendix B. The sense for the method is that it would diffuse the divergence similar to Yabe's pressure Poisson equation. The velocity field should be closer to satisfying divergence constraint.
4. Implementing a turbulence model and/or wall laws. A more sophisticated turbulence model such as the $(k - \epsilon)$ turbulence model could be implemented to better represent the fluid flow.

The extensions of the current work are listed as follows:

1. Develop a complete model of the shot sleeve including cycles for liquid and air flow, the plunger and shot sleeve walls. Include the shot sleeve cylinder and

plunger mechanism in the thermal analysis. Nitsche's method as described by Hansbo [72] could be used on the interface between liquid and solid.

2. Fluid flow in the runner would be the next phase of the filling of die cavity. This is slug flow and the methodology used in the shot sleeve analysis could be applied.
3. Fluid flow from the runner through the gates into the casting cavity. The flow of molten metal through the gate is characterized by its thin cross-section and high speed. Usually the gate is 0.5-1 mm thick and 10 mm long. When liquid metal accelerates from the runner to the gate, the phenomena of shock wave or water hammer may appear. The velocity of liquid could reach up to 50 m/s, which is two orders higher than the slow shot velocity. That means the Brinkman number is in the order of 0.01. If phase change is also involved, i.e., mushy liquid occurs, viscous heating may need to be considered. At the same time, the pressure can be estimated by Poiseuille flow through the gate, which is about 4000 Pa if the viscosity is 10^{-3} Pa·s. The exponential increase of the viscosity by solidification may impose some difficulty on the filling of die cavity because large pressures are necessary.
4. Filling of die cavity. The filling of die cavity is characterized by high velocity and a large free surface area. Mesh distortion could be very large.

- (a) In this case, it would be better to use the droplets or particles to represent the liquid domain. The mass particle method of Yserentant [73] could be a good approach. In this thesis, Yserentant's mass particle method was fully implemented. However, too many time steps were needed for time integration to use it in the shot sleeve.
 - (b) The velocity field could be solved by the Incompressible Flow Solver with the STL file of casting being a constraint. Instead of moving the nodes the particles can be advected by the velocity field and a new domain for the liquid can be determined by the advected particles.
 - (c) A staggered mesh or a mesh with 6-node brick elements could be tried because the divergence based on the faces of an element seems to have more physical meaning. In addition, the staggered mesh and 6-node bricks better capture vorticity. While filling the cavity, air can be trapped and compressed such that it reaches very high pressures. The stored energy in this compressed air could have a large effect in the filling of the cavity and the quality of the casting.
5. The best opportunity to maximize production rate is to optimize the cooling process by optimizing the position of cooling lines and optimizing the spray cooling of the die cavity surface.

Chapter 6

Conclusions

The flow and heat transfer of molten metal inside the shot sleeve of a cold-chamber die casting machine during the slow shot were analyzed by solving a coupled problem governed by the conservation of mass, momentum and energy using a three-dimensional (3-D) finite element method. This research is the first to solve the 3D transient Navier-Stokes equations to compute evolution of a wave in the shot sleeve including breaking waves. It is the first to solve the energy equation with solidification coupled to the transient Navier-Stokes equations. The software gives designers a clearer overall picture of the slow shot process and enables them to optimize the injection parameters.

The software was verified by solving several well known fluid flow and heat transfer problems with known solutions or experimental results. The effects of main param-

ters such as the inner diameter of a shot sleeve, the initial fraction filled and the acceleration on the critical slow shot velocity were investigated and the results attained numerically match the analytical results. The wave patterns were simulated and matched qualitatively well with the experimental results. The fluid flow and thermal analyses were conducted for the cylindrical shot sleeve. The following conclusions can be drawn:

1. The numerical experiments at the symmetry plane of the cylindrical shot sleeve suggest that the critical slow shot velocity is influenced by the inner diameter of a shot sleeve, the initial fraction filled and the acceleration of the plunger.
 - As the inner diameter of shot sleeve increases, the critical velocity increases. This result matches the analytical solutions. This suggests that shorter, fatter shot sleeves be used.
 - As the initial fraction filled increases, the critical velocity decreases. For lower initial fractions filled (≤ 0.3) the tendency to form a breaking wave is very high. For this reason a lower initial fraction filled is not recommended.
 - As the acceleration increases, the critical velocity decreases although the magnitude of the effect is small. The acceleration does have a significant effect on the shape of the wave, i.e., the thickness or width of the wave increases as the acceleration decreases. A stable thick wave leads to mini-

mum or no air entrapment.

2. Since data acquisition in the shot sleeve is difficult, the use of the a 2-D analysis to provides a good approximation to the optimal plunger profiles for process development could be valuable. The 2-D analysis is very fast and usually takes 12 minutes to perform.
3. All known wave patterns in shot sleeve flow have been simulated and they match the experimental results. In addition, one new wave pattern was found.
4. Air entrapment in the shot sleeve is determined by the plunger velocity, the acceleration, the initial fill level, and the inner diameter of a shot sleeve. A plunger profile with the critical slow shot velocity and appropriate acceleration will entrap minimal air or no air. Velocities above and below the critical velocity will increase air entrapment.
5. The flow analysis of molten metal in cylindrical shot sleeve was conducted and wave profiles for different plunger profiles were obtained. The 2-D and 3-D fluid flows do show some similarities.
6. Solidification does occur during the slow shot of a die casting. But the effect of solidification on the following fast shot could be small because it only occurs near the plunger and this solid may not enter the die cavity during the filling of die cavity.

7. Computation times and the computer hardware resources required to run the 3-D simulations discussed in the research were modest. All simulations were run on a Pentium IV 1.8 GHz PC with 2 Gb RAM. The simulation times for the 3-D transient analysis of fluid flow and heat transfer are about six hours.

Appendix A

Uzawa's Algorithm

Uzawa's Algorithm solves the 2×2 system of equations including the case with $\mathbf{C} = \mathbf{0}$

$$\begin{bmatrix} \mathbf{M} + \mathbf{K} & \mathbf{B}_{\text{div}}^T \\ \mathbf{B}_{\text{div}} & \mathbf{C} \end{bmatrix} \begin{bmatrix} \bar{\mathbf{v}} \\ \bar{p} \end{bmatrix} = \begin{bmatrix} \bar{\mathbf{y}} \\ \bar{w} \end{bmatrix} \quad (\text{A.1})$$

It augments the first equation with the penalty operator $\mathbf{K}_k = \Pi_{e_i=1}^{n_e} \int_{\Omega_{e_i}} r \nabla(\nabla \cdot \mathbf{v}) d\Omega$.

The factor r can be interpreted to be a numerical bulk modulus times the time step length $\kappa_b \Delta t$. The algorithm can be summarized by the following steps [66]:

Step 1. Assume initial values of velocity field $\mathbf{v}^0(t_{n+1})$ and pressure field $p^0(t_{n+1})$.

Step 2. For Newton-Raphson iteration $n+1$ solve conservation of mass and momentum equations for corrections to velocity $d\bar{\mathbf{v}}^{n+1}$ and pressure $\bar{p}^{n+1}$.

$$\begin{aligned}
[\mathbf{M} + \mathbf{K}_\mu + \mathbf{K}_k] [d\bar{\mathbf{v}}] &= -[\mathbf{M} + \mathbf{K}_\mu + \mathbf{K}_k] [\bar{\mathbf{v}}] + \\
&\quad [\mathbf{F}_{\text{ext}}(t_{n+1}) + \mathbf{F}_{\text{ext}}(t_n)]
\end{aligned} \tag{A.2}$$

Step 3. For Newton-Raphson iteration $n+1$ add corrections to velocity and pressure.

$$\begin{aligned}
[\bar{\mathbf{v}}]^{n+1} &= [\bar{\mathbf{v}}]^n + [d\bar{\mathbf{v}}]^n \\
p^{n+1} &= p^n - r \nabla \cdot \bar{\mathbf{v}}^{n+1}
\end{aligned} \tag{A.3}$$

Step 4. If this Newton-Raphson iteration has not converged, go to step 2.

Appendix B

Condensing a 2×2 System at Element Level

We write the element 2×2 system at the element level in the form.

$$\begin{bmatrix} \mathbf{K}_{vv} & \mathbf{K}_{vp} \\ \mathbf{K}_{pv} & \mathbf{K}_{pp} \end{bmatrix} \begin{bmatrix} \bar{\mathbf{v}} \\ \bar{\mathbf{p}} \end{bmatrix} = \begin{bmatrix} \mathbf{w}_v \\ \mathbf{w}_p \end{bmatrix} \quad (\text{B.1})$$

The entries in the 2×2 system for the Stokes problem or for static elasticity are

$$\begin{aligned} \mathbf{K}_{vv} &= \int_{\Omega_{e_i}} \nabla \mathbf{R}^T D \nabla \mathbf{R} d\Omega \\ \mathbf{K}_{vp} &= \int_{\Omega_{e_i}} (\nabla \cdot \mathbf{R})^T \mathbf{R}_p d\Omega \\ \mathbf{K}_{pv} &= \int_{\Omega_{e_i}} \mathbf{R}_p^T (\nabla \cdot \mathbf{R}) d\Omega \end{aligned}$$

$$\mathbf{K}_{pp} = \int_{\Omega_{e_i}} \mathbf{R}_p^T \frac{1}{\kappa_b} \mathbf{R}_p d\Omega$$

The 2×2 system can be condensed to

$$\tilde{\mathbf{K}}_{vv} = \mathbf{K}_{vv} - \mathbf{K}_{vp} \mathbf{K}_{pp}^{-1} \mathbf{K}_{pv}$$

$$\tilde{\mathbf{w}}_v = \mathbf{w}_v - \mathbf{K}_{vp} \mathbf{K}_{pp}^{-1} \mathbf{w}_p$$

For the Q1-P0 8-node brick element, the basis functions for piecewise constant pressure are $\mathbf{R}_p = \{1\}$ and the matrix $\mathbf{K}_{pp}$ evaluated with 1-point Gaussian integration and its inverse are

$$\begin{aligned} \mathbf{K}_{pp} &\equiv \int_{\Omega_{e_i}} \mathbf{R}_p^T \frac{1}{\kappa_b} \mathbf{R}_p d\Omega = \frac{8 \det J}{\kappa} \\ \mathbf{K}_{pp}^{-1} &= \frac{\kappa_b}{8 \det J} \end{aligned}$$

and the other three matrices are evaluated with $2 \times 2 \times 2$ Gaussian integration. For a brick with piecewise linear pressures, such as the 15-node brick, the pressure basis functions are $\mathbf{R}_p = \{1, x, y, z\}$ and the pressure DOFs are $\{p, p_x, p_y, p_z\}$.

$$\mathbf{K}_{pp} \equiv \int_{\Omega_{e_i}} \begin{bmatrix} 1 \\ x \\ y \\ z \end{bmatrix} \frac{1}{\kappa_b} \begin{bmatrix} 1 & x & y & z \end{bmatrix} d\Omega$$

In this case, the inverse of this 4×4 matrix could be computed. Another numerical method is to solve the following system for the 4×45 matrix $\mathbf{y}$. This requires one solve for each of the 45 columns $\mathbf{y}$.

$$\mathbf{K}_{pp} \mathbf{y} = \mathbf{K}_{pv}$$

$$\mathbf{y} = \mathbf{K}_{pp}^{-1} \mathbf{K}_{pv}$$

$$\mathbf{K}_{vp} \mathbf{K}_{pp}^{-1} \mathbf{w}_p = \mathbf{K}_{vp} \mathbf{y}$$

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