SIMULATION OF NON-RETURN VALVE CLOSURE IN A
THIXOMOLDING PROCESS UTILIZING A MAGNESIUM
ALLOY

by

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Robert Da Silva

Abstract

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The objective of this thesis is to create a simulation model for a non-return valve in a thixomolding process with a magnesium alloy as the material. Modeling goals are to provide insight into the valve operation, as well as design optimization avenues. Model development first involved validation through element size and time step convergence tests. The next step involved determining the role of various operation parameters such as the viscosity, density and pressure conditions. The final step was to evaluate the model adaptability to valve geometry alteration. The results showed good convergence in the validation portion. The pressure forces generated due to valve body movement and flow of the fluid pass the ring component were the dominant force governing the valve movement. Density measured the strength of the link between the valve body and the ring, governing the amount of momentum transfer. As for viscosity, it was shown to acts as damping to the system. Finally, alterations to the geometry were shown to directly affect the valve closure speed. Improvements to the model are possible by making the viscosity temperature dependent, as well as using experimental results to further verify the physical model.

Table of Contents

Abstract	iii
Table of Contents	iv
List of Figures.....	vi
List of Tables	viii
Acknowledgments.....	ix
Nomenclature	x
Chapter 1 Introduction	1
Chapter 2 Introduction to Thixomolding	6
Thixomolding Machine Components	6
Hopper	7
The Barrel	7
Screw	7
Non-Return Valve	9
End Cap and Nozzle	11
Clamping Unit and Mold.....	12
Thixomolding procedure.....	14
Process Variables.....	15
Chapter 3 Background Theory	18
Governing Equations.....	19
Continuity Equations	20
Momentum Equations	20
Energy Equations	21
General Transport Equation	22
Finite Volume Method	23
FLUENT Theory and Application.....	29
Boundary Conditions	30
Physical Properties.....	32
Dynamic Mesh	32
Modeling Solidification and Melting.....	35
User Defined Files	37
Chapter 4 Valve Modeling Procedure	39
Valve Geometry.....	39
Geometric Simplifications	41
Meshing Procedure	43
Mesh Motion	45
Case Variations Modeled.....	50
Flow Material Properties.....	51
Chapter 5 Results	53
Model Validation	53
Steady State Analysis	53
Mesh Selection	61

Time Step Reduction.....	64
Effect of Ramp-up.....	68
2D Axisymmetric compared to full 3D model.....	72
Valve Operation Results.....	75
Baseline Results.....	76
Plastic Material Properties	80
Effect of Thermal Properties.....	83
Barrel Pressure	88
Input Velocity Profile Alterations	92
Design Alterations.....	95
Ring Rear Angle Geometry Alterations.....	95
Ring Front Angle Geometry Alterations.....	97
Chapter 6 Conclusion	101
References	107
Appendix	111
UDFs	111
Valve body Motion.....	111
Ring motion.....	111

List of Figures

Figure 1-1: Effect of Barrel Temperature on Solid phase content. [Lohmuller, 24].....	2
Figure 2-1: Schematic of Thixomolding Machine. [19].....	6
Figure 2-2: Elements of an Thixomolding Machine Screw. [Olmsted, 28].....	8
Figure 2-3: Schematic of Ring Type Non Return Valve [Olmsted, 28].....	9
Figure 2-4: Schematic of Ball Check valve. [Olmsted, 28].....	11
Figure 2-5: Nozzle, Valve and End Cap Assembly [Olmsted, 28]	12
Figure 2-6: Schematic of Clamping Unit and Mold. [Olmsted, 28].....	13
Figure 2-7: Stages of Thixomolding Cycle. [Olmsted, 28].....	14
Figure 3-1: Finite Control Volume Fixed in Space. [Anderson, 5].....	19
Figure 3-2: 1D Finite Control Volume Volume.....	24
Figure 3-3: 2D Finite Control Volume. [Versteeg, 39].....	24
Figure 3-4: FLUENT Program Structure [FLUEN, 12].....	29
Figure 3-5: Illustration of Spring-Base smoothing. [FLUENT, 12].....	34
Figure 3-6: Calling sequence diagram for a UDF [FLUENT, 12].....	38
Figure 4-1 - Valve Assembly	40
Figure 4-2 - Valve Components. The Valve Body is on the Left and Ring on the right.	40
Figure 4-3 - Generation of the 2D Axisymmetric Model.	42
Figure 4-4 - Plane Cutout of 3D Mesh.....	44
Figure 4-5a: Frame of Mesh Progression through time ($t=0$ sec).	46
Figure 5-1: Valve Geometry Including Gap between Ring and Barrel. Top illustrates the entire model, and below is a closer view of the highlighted area.....	54
Figure 5-2: Quadrilateral Mesh	54
Figure 5-3: Triangular Mesh.....	55
Figure 5-4: Outflow Velocity	56
Figure 5-5: Convergence of Force on Ring.....	57
Figure 5-6: Pressure Contours	58
Figure 5-7: Closer Examination of Corner Pressure Contours.....	59
Figure 5-8: Velocity Vectors about Corner.	59
Figure 5-9: Velocity Vectors of the Flow in the Gap.	60
Figure 5-10: Various Element Sizes	61
Figure 5-11: Variation of the Force on Ring due to Different Element Sizes.....	62
Figure 5-12: Variation of the Ring Velocity due to Different Element Sizes	63
Figure 5-13 Force on Ring Profiles with Varying Time Step Size.....	65
Figure 5-14 Force on Ring Profile with Very Small Time Step Sizes.	65
Figure 5-15: Close Inspection of the Force Profile with various Time Step Sizes.....	67
Figure 5-16: Ring Velocity with Various Time Step Sizes	67
Figure 5-17: Valve Assembly Velocity Profiles.	68
Figure 5-18 Force on Ring with Various Ramp-up Profiles.....	69
Figure 5-19: Ring Velocity with Various Ramp-up Profiles.	70
Figure 5-20: Force on Ring with Various Ramp-up Profiles with time correction.....	71
Figure 5-21: Ring Velocity with Various Ramp-up Profiles with time correction.	72
Figure 5-22: Force on Ring Profile for 2D axisymmetric and full 3D model.....	72
Figure 5-23: Ring Velocity Profile for 2D axisymmetric and full 3D model.	73
Figure 5-24: Velocity Contours in 3D model.	74

Figure 5-25: Velocity Contours using 2D axisymmetric model.....	74
Figure 5-26: Baseline Force Profile.	76
Figure 5-27: Pressure Contours Over Entire Domain.	77
Figure 5-28: Velocity Contours Over Entire Domain.....	78
Figure 5-29: Velocity Vectors at Rear of Ring.....	79
Figure 5-30: Pressure Contours Near Rear of Ring.....	79
Figure 5-31: Baseline Ring Velocity Profile.	80
Figure 5-32: Force on Ring with Different Material Properties.....	82
Figure 5-33: Ring Velocity with Different Material Properties	82
Figure 5-34: Temperature Contour at Start of Valve Closure.....	84
Figure 5-35: Liquid Fraction near the Rear Seat.....	85
Figure 5-36: Force on Ring including Thermal Effects.	86
Figure 5-37: Ring Velocity including Thermal Effects	86
Figure 5-38: Change to Temperature Contours due to Valve Motion.....	87
Figure 5-39: Nozzle Effect on Pressure Field.	88
Figure 5-40: Force on Ring with various Back Pressures.	89
Figure 5-41: Ring Velocity with Various Back Pressures.....	90
Figure 5-42: Velocity of Leakage flow (Back Pressure cases).....	91
Figure 5-43: Barrel Injection Velocity (Back Pressure cases).	91
Figure 5-44: Various Stud Velocity Profiles.....	92
Figure 5-45: Force on Ring with various Input Profiles.	93
Figure 5-46: Ring Velocity with various Input Profiles.....	94
Figure 5-47: Force on Ring Profiles with Rear Angle Alterations.....	96
Figure 5-48: Ring Velocity Profiles with Rear Angle Alterations.	96
Figure 5-49: Ring Geometry with a Front 10° Change.	97
Figure 5-50: Force on Ring Profiles with Front Angle Alterations.....	98
Figure 5-51: Ring Velocity Profiles with Front Angle Alterations.	98
Figure 5-52: Drag Results of Ring with Front 10° Alteration and modeled in 3D.....	99
Figure 5-53: Velocity Profile of Ring with Front 10° Alteration and modeled in 3D.	99

List of Tables

Table 1-1 - Process Variables	15
Table 3-1: Properties of Magnesium Alloy AZ91D.....	52
Table 3-2: Properties used to simulate various Plastic Polymers.....	52
Table 4-1: Common Injection Molding Thermoplastics Density.....	81

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Nomenclature

Acronyms

ABS	Acrylonitrile Butadiene-Styrene
CFD	Computational Fluid
CV	Control Volume
FDM	Finite Difference Method
FEM	Finite Element Method
FVM	Finite Volume Method Dynamics
GPPS	Polystyrene
IM	Injection Molding
PA	Nylon
PC	Polycarbonate
PP	Polypropylene

English Symbols

A	cell area
A_{mush}	mushy zone damping term
a	acceleration
C_p	
dt	infinitesimal time step
e	internal energy
F, F_{net}	net force
F_{viscous}	represents the total effect of the viscous forces on CV
f	net body force per unit mass exerted in the fluid inside the CV
H	enthalpy
ΔH	corrected latent heat
h	sensible enthalpy
h_{cell}	cell height
h_{ideal}	ideal cell height
$L, \Delta H$	latent heat
m	mass
N, S, E, W, P	centroid and nodal points on FVM Grid
n, s, e, w	cell boundary points on FVM Grid
Pe	pecllet number
p	pressure
$\dot{Q}_{\text{viscous}}$	rate of heat addition to the CV due to viscous effects
$\dot{q}$	volumetric rate of heat addition per unit volume
S	surface of the control volume
S_{ϕ}, S	source term
T	temperature
T_{liquidus}	melting temperature

T_{solidus}	solidification temperature
t	time
u, v, w	velocity components (Cartesian x, y, z directions)
u^*, v^*, p^*	initial guess for u, v, p used in iterative solution process in FVM
u', v', p'	correction values for u, v, p used in iterative solution process in FVM
V	velocity
V	volume
V_g	grid velocity
$\dot{W}_{\text{viscous}}$	rate of work done on CV due to viscous forces
$\Delta x, \Delta y$	width and height of the control volume

Greek Symbols

α_c	cell split factor
β	liquid fraction
Γ	diffusion coefficient
δ	distance between grid points on FVM grid. Subscripts denote which points.
ρ	density
ϕ	represent a general variable per unit mass inside the CV

Chapter 1 Introduction

Injection Molding has been around for quite some time now, dating back to 1868. At the time, John Wesley Hyatt's invention profoundly increased manufacturing efficiency and to this date the technology is still evolving. There are two main types of injection molding (IM) machines, which are Die Cast and plastic. The main difference between the two is essentially the materials they use, in that the die cast utilizes molten metals and plastic IM uses plastics polymers. The common link is the IM process itself, whereby the material, be it metals or plastics, is first melted into liquid form then injected into the mold. A new variation of the technology has recently emerged in which the material is not melted completely, but rather is injected in a semi-solid state. This process is known as thixomolding. The material utilized here is always a molten metal and more often than not a magnesium alloy. Thixomolding is still in its infancy stage, being first proposed in the mid 70's. Throughout the 80's the technology was researched extensively and it was not until the 90's that the first Thixomolding IM machines were built. Actual industrial usage has only begun within the last five years or so. The rapid development would suggest that the technology has some strong advantages; however, being that it is still relatively new means the process still has some areas where improvement can be made.

The main advantage of injecting a semi-solid material involves a very important property, viscosity. If viscosity is low, the flow of material during injection may be turbulent which can lead to the creation of air pockets and increased porosity, which means more defective parts. On the other hand, high viscosity means the material is more difficult to move and so it is more difficult to reach the extremities of the mold before solidification.

By utilizing a semi-solid state, viscosity is no longer a hindering variable but rather an independent one. The designer can get an optimal viscosity by simply adjusting the injection temperature, thereby adjusting the solid phase content ratio within the melt. The shearing forces introduced between the solidus and the liquidus particles are the cause of increased viscosity. Figure 1 depicts the solidus content as a function of temperature for a magnesium alloy. Here, it is apparent how a low temperature melt, such as the first picture in figure 1, is more restricted during flow than the one at a higher temperature, like the last picture in figure 1-1. The typical barrel temperature for thixomolding usually fits in the range of 580 °C to 595 °C for magnesium alloys. In short, the main advantage of thixomolding is that it

Figure 1-1: Effect of Barrel Temperature on Solid phase content. [Lohmuller, 24]

allows for laminar flow, even if high injection speeds are used.

The laminar flow property leads to other advantages, predominantly caused by the improved part quality. The reduced porosity means less defective parts are generated, thus greater product consistency and repeatability. Also, the smooth mold filling improves surface quality and so less post-process machining is required. Furthermore, the laminar flow allows for a greater variety of part wall thickness, reaching as low as 0.6 mm. Another advantage gained by utilizing the thixomolding process is that the operating temperatures are lower, anywhere from 30°C to 125°C. This leads to lower operating costs and quicker cooling times. Finally, there is no flux, sludge or dross, and because the process is self-contained and protected by argon gas, the excess material can simply be reused.

In addition to the advantages gained by the thixomolding process, there are several benefits that arise due to the use of magnesium alloys. Firstly, the stiffness to weight ratio of magnesium alloys is better than both aluminum and plastics, yet the part is weldable and heat treatable. Also magnesium is very easy to machine. Secondly, it is the only metal to have inherent damping, yielding quieter operation of equipment with magnesium housings. Thirdly, magnesium alloys have inherent electromagnetic shielding, lending themselves for use in the electronics industry. Lastly, magnesium is dimensionally stable, meaning the shape of the part does not alter after cooling is complete due to such factors as aging. When all is said and done, thixomolding of magnesium alloys allows for the production of thinner and higher quality parts ideal for use in the electronics, automotive and various other consumer products.

On the other hand, there are disadvantages to thixomolding. To the forefront is that the experience base is limited and not yet developed, thixomolding is still relatively new. A more important disadvantage is the reduced tool life. The consistency of the melt is similar to that of sand paper, and so the increase abrasive quality leads to increase wear of the

injection machine components. The higher viscosities require greater cavity pressure, up to twice as much as die cast. Therefore, a higher clamping force in the mold is required and there is a higher probability of residual stresses being created. As for the material itself, magnesium alloys are more expensive than aluminum and plastic counterparts.

Overall the advantages of thixomolding outweigh its disadvantages. Furthermore, most of the disadvantages are such that, with more research, they can be eliminated or at least minimized. Optimizing all aspects of thixomolding is beyond the scope of this thesis, instead one component of a thixotropic injection molding machine will be scrutinized, namely, the non-return check valve. One goal is to determine the effect of various operating variables, for instance, the effect of viscosity on the effectiveness of the valve. Which variable chosen and how they are altered will have a link to the thixotropic behaviour of the melt. The second objective is to determine flaws in the design or to outline areas in which the design can be improved and implement possible changes in a set of new tests, in essence, attempt to improve the valve design.

Currently, Thixomolding machines are adapted versions of plastic injection molding equipment. To expect them to perform just as efficiently when dealing with a harsher material is unrealistic. When attempting to improve operation of a component, it is important to determine the effect of the material on the valve, which relates to the first goal. The variables to be altered include viscosity, density, temperature, and certain pressures. Simulaion will be accomplished through the use of computer modeling utilizing FLUENT. The computer model establishes the variation of the internal forces and the resulting velocities of the moving components. In addition, the mass flows of the injected melt and of the leakage are monitored. The first step, however, is to give the model some validation.

Once a knowledge base of the valve operation is established, it is then possible to address the issue of flaws. For example, while monitoring the mass flow of the leakage, one can conclude whether too much of the melt is escaping. Then the leakage can be focused on in an attempt to minimize this variable. The proposed solutions will come in the form of suggestion of how to alter certain operating variables whose effect is to minimize the proposed flaw. For instance, one can show how altering the injection speed profile helps reduce leakage. The following step would be to apply some optimization technique to improve operation efficiency. Actual optimization of the valve operation is beyond the scope of this thesis, instead the effects of various variables will be documented. In the end, the hope is to provide insight into how to improve tool life and efficiency.

Before one can delve into improving the technology, it is important to become familiarized with the machinery involved and the thixomolding process. Despite the fact that only the check valve is being addressed, it is still important to understand how the entire machine works because changes that affect one component will affect the others as well. Furthermore, the other components may place restrictions on the valve in question. One must outline the driving variables and the dependent counterparts. The next logical step is to set down some basics of computational fluid dynamics (CFD), its limitations and how the valve was modeled. Once the background theory has been established, the natural progression is to provide the model validation and valve operation results. This will be followed by the results and discussion pertaining to design improvements. Finally, a conclusion with a discussion of possible future work will be presented.

Chapter 2 Introduction to Thixomolding

Although the concept behind thixomolding is simple, the machinery is quite complex and there are many process variables to contend with. The main components of the machine include the Hopper, the Screw, the Barrel, Heater Bands, the Non-Return Valve, the Nozzle, and the Mold. As for the process variables, they can be separated into five main categories, each with several variables in that category. The five sets of variables are Temperature, Time, Speed, Pressure and Stroke. Not all of the variables are controllable directly; with some, the manipulation of a variable is a consequence of altering other variables. In other words, they are controlled indirectly.

Thixomolding Machine Components

As previously mentioned the thixomolding machine is comprised of many parts. The breakdown of set components is shown in figure 2-1.

Figure 2-1: Schematic of Thixomolding Machine. [19]

Hopper

Simply put, the Hopper is the opening through which the material of choice is loaded into the machine. The material, Magnesium chips in this study, enters the machine and into a conveyor system, usually pneumatic. Here, dryers remove moisture from the chips which then proceed to a feeder. At this point, additives may be added. For magnesium, it is where argon gas is added, which reduces oxidation. The feeder transports the prepared chips to the opening in the barrel.

The Barrel

The Barrel (or cylinder) is a tube, usually steel, that houses several other components of the machine. The outside the barrel is equipped with heater bands, whose role is to provide the energy required to melt the magnesium chips. However, they do not provide all of the energy; some is generated by the shearing forces of the rotating screw. Note, these bands also heat the nozzle. Furthermore, the barrel is equipped with thermocouples, located between the heater bands, whose role is to determine the temperature along its length. The inside of the barrel is lined with a wear resistant material, such as a tool grade steel.

Screw

One of most complicated parts in the thixomolding machine is the screw. Figure 2-2 provides a detailed schematic of this component. First off, the screw is broken down into sections, the Shank and Flighted Length. The shank is designed to couple the screw to the drive unit, which provides the rotation motion of the screw. The Flighted Length makes up 80% of the entire screw length and is responsible for moving the melt forward, with the help of screw slots. The hopper feed entrance coincides with the start of

Figure 2-2: Elements of an Thixomolding Machine Screw. [Olmsted, 28]

the Flighted Length just after the Shank portion, labeled Pocket in figure 2-2.

The Flighted Length is then divided into three subsections, Feed, Transition and Meter portions. In the feed section, the material begins to melt but is mostly comprised of solid chips. As the material is moved forward, into the transition portion, it becomes compressed and so the material does most of its melting here. The compression is caused by the increasing diameter of the screw, and for this reason the transition section is also known as the compression zone. The final zone is the meter, which again has a constant screw diameter. The meter continues to move the melt forward, evening out the temperature distribution of the melt. The heated material then passes through a non-return valve, building up the pressure as it accumulates.

When designing a screw, there are several key variables one must balance. The screw has a pivotal role in determining the melt temperature and pressure, so its design is critical, especially when it comes to thixomolding machines. These variables include the length-to-diameter ratio, the compression ratio, screw profile (i.e., lengths of the subsections), and the helix angle. Categorization of the screws is done using these variables.

Non-Return Valve

The Non-return valve is also one of the most intricate components of the thixomolding machine. However, its design is not machine specific, one design works with almost all screw variations. The valve itself is threaded to the end of the screw and its main purpose is to stop backward flow of melt once the material has passed the end of the screw. There are a few design variation of the valve, but their role remains the same. Figure 2-3 illustrates one of the more common models, the Ring Valve.

Figure 2-3: Schematic of Ring Type Non Return Valve [Olmsted, 28]

The Ring valve illustrated is a three piece configuration, the Rear seat, Ring and Stud. The ring is the component responsible for opening and closing the valve through its movement forward or backwards, respectively. When in the forward position, the melt passes through groves cut into the stud, labeled flutes. No such groves exist in the rear seat, so that, when the ring is in the backward position, flow is blocked. The pressure in the barrel is what causes the ring to move. Thus, if the pressure is higher in front of the flute,

the valve closes to prevent backflow. The pressure itself is generated by the movement of the screw. So, if the screw moves forward, the pressure builds up in front of the valve and again it closes. The gap between the ring and the barrel is very small, on the order of 0.0015 to 0.038 inches, in comparison to a 2 inch ring (common barrel size). Therefore, no appreciable amount of melt leaks through that gap.

Failure of the valve occurs in a couple of ways, one being when the barrel becomes worn the ring is allowed to expand (due to large internal pressures) and at some point it will break. Furthermore, the efficiency of the ring valve decreases as the valve itself wears. The most common area of wear is the contact point between the ring and one side of the stud. The reason for increased wear here is the contact friction generated by the rotating screw rubbing against the ring. There is a four piece valve available in which the stud is split into a stud and a front seat. Basically, if the valve becomes worn, only the front seat must be changed and not the entire stud. Another ring valve variation that attempts to address the wear issue is a locking ring valve. Here, the ring locked to the stud when the valve is closed so that it rotates with the rest of the screw, eliminating the wear problem altogether.

A second valve design also commonly used is the ball check valve. It operates on similar principles as the ring valve; however, the ring is replaced by a ball. Figure 2-4 shows a schematic of a ball check valve. The ball moves forward and backwards due to pressure variations, which in turn open and close the valve. Another valve design, less common, is the spring valve, in which a spring is attached to a piston and it compresses and expands to open and close the valve, respectively. The ball and ring valve are the most common though. The ring valve is freer flowing so that in cases where the melt is sensitive to shear the ring valve is used.

Figure 2-4: Schematic of Ball Check valve. [Olmsted, 28]

End Cap and Nozzle

As the name suggest, the end cap is a cap at the end of the barrel. One of its purposes is to withstand the large internal pressures generated during the injection cycle. The other function of the end cap is to provide a mounting surface for the nozzle. The nozzle is threaded into the end cap as illustrated in figure 2-5. The nozzle is a tube which provides a mechanical and thermal connection from the hot barrel to the much cooler injection mold with a minimum pressure and thermal loss. There are three kinds of nozzle designs, one with an open, unrestricted channel. The second has a valve which closes with diminishing injection pressure and the third has a manual shutoff which is either pneumatically or hydraulically closed.

Figure 2-5: Nozzle, Valve and End Cap Assembly [Olmsted, 28]

Clamping Unit and Mold

The clamping unit has several simple self explanatory functions which are listed below:

1. Hold the mold.
2. Close the mold.
3. Keep the mold closed when under pressure of injection.
4. Open the mold to allow part ejection
5. House ejection system.

A schematic is shown in figure 2-6. The clamping mechanism is usually hydraulic and comes in two forms, each with its pros and cons. The first utilizes a single hydraulic ram in direct contact with a moving plate. The other also uses a single hydraulic ram but it is indirectly attached to the moving plate through a system of linkages. The linkages are used to provide mechanical advantage, requiring a smaller hydraulic ram. The ejector system can

Figure 2-6: Schematic of Clamping Unit and Mold. [Olmsted, 28]

be either mechanical or pneumatic. In the mechanical system, there are stationary rods that pass through holes in the moving plate of the mold. As the plate moves back, the rods press against the part, ejecting it from the mold.

In regards to the mold, it is the most complicated part of the thixomolding machine. A detailed description of the components and design is not required when considering the operation of the non-return valve, and so is beyond the scope of this thesis. Briefly put, the mold is comprised of two halves each containing gates, cooling lines, venting lines and ejector holes. Gates are the paths that the melt travel to on it path to the mold cavity, that is the part itself. Cooling lines are used to strategically remove heat from the mold to achieve proper solidification of the melt. Venting lines are paths which allow the air in the cavity to escape. Finally, part ejection is accomplished either mechanically with ejector pins or pneumatically.

Thixomolding procedure

From the point of view of the part, there are three stages in the thixomolding process, mold filling, solidification (or cooling) and part ejection. For each stage, the screw performs certain tasks to make the entire cycle possible. The cycle timing is illustrated in figure 2-7. When the screw is moved forward, it pushes the accumulated melt into the

Figure 2-7: Stages of Thixomolding Cycle. [Olmsted, 28]

Mold, known as the injection phase. At this point the screw is not rotating. The time at which the screw moves forward is slightly longer than the mold filling time to ensure all the air in the mold escapes, at which point some melt will escape through the air vents.

While the part is cooling, the screw holds its position for the first portion of time. Here, the pressure must be maintained until sufficient solidification occurs such that the part can keep its shape. As the part continues to cool, the screw begins to rotate and melt begins to accumulate again in preparation for the next cycle, hence the label screw recovery. The final step for the screw is dwelling time in which it waits for any final cooling and the ejection of the part. The cycle is then ready to begin again.

One should note that the majority of time is spent in part cooling. The cooling time is a function of part thickness and, to a lesser degree, the desired mechanical properties.

Process Variables

There are literally dozens of process variables each interconnected, making optimization very difficult. As mentioned earlier, the best starting point is to organize the variables into categories. Table 1.1 lists the five main categories and some of the variables that fall it those categories.

<i>Temperature</i>	<i>Times</i>	<i>Speeds</i>	<i>Pressure</i>	<i>Strokes</i>
Melt	Ejection	Injection	Holding	Melt cushion
Barrel	Mold Close	Screw	Injection	Screw
Mold Surface	Mold Open	Screw Return	Hydraulic Back	Mold Open
Coolant	Cooling	Ejection	Ejection	Change Over
	Cycle		Mold Safety	
	Screw Recovery			
	Holding Press.			

Table 2-1 - Process Variables

Some of these variables are not directly controllable, and thus are further labeled as controllable of consequential variables, referring to whether they are controlled directly or indirectly, respectfully. Knowing the relationships between variables is important to first know how to adjust consequential variables and also to know what options are available to make the desired adjustments.

In regards to temperature variables, the most important is the melt or material temperature. It determines the consistency of the melt and is especially important in thixomolding. This variable is a perfect example of a consequential variable in that it is not controlled directly. It is a result of interaction between the screw rotation speed, the back pressure, the barrel temperature and the injection cycle timing. The barrel temperature, however, is controllable by adjusting the power sent to the heater band. The mold

temperature and coolant temperature affect how the part cools, as well as the cooling rate of the melt.

All of the timing variables were essentially discussed in the previous section and thus require little mention here except that the cycle time is the combination of all other time variables.

One of the most important speed variables is the injection speed, which represents the rate at which the melt is injected into the mold. The injection speed is directly related to the cooling variable in determining the final properties of the part. Furthermore, the injection speed is dependent on having sufficient pressure in the barrel to maintain the desired speed. Inconsistent mold filling arises from insufficient barrel pressure. Ultimately, the injection speed is regarded as a controllable variable. The two speed control variables for the screw are the rotation speed and recovery speed. Control of the screw has a direct influence on the melt temperature and to a small degree an influence on the cycle timing.

The three prominent pressure variables are Injection, Holding and Hydraulic back pressure. Injection pressure, as mentioned earlier, is important to injection speed, and so maintaining a constant pressure value is desirable. However, injection pressure is not a directly controllable variable, otherwise known as a consequential. It is affected by the melt temperature, the viscosity characteristics, injection speed, surface temperature of the mold and the distance the melt is required to travel. Holding pressure is the barrel pressure maintained during holding time and is a controllable variable which has a direct relation to mold cooling. The hydraulic back pressure is the barrel pressure during the screw recovery period.

The stroke variables are related to the distance traveled by certain components. For instance, the screw stroke is the linear distance the screw travels due to injection. It is

directly related to the size of the part and the melt cushion. The melt cushion is the excess melt left in the barrel after the injection period. Finally, the changeover position variable is the screw position point at which the pressure in the barrel changes from injection pressure to holding pressure.

Chapter 3 Background Theory

The theory base of CFD is very complex; it involves highly nonlinear and strongly coupled governing equations. Therefore, the solution algorithms used by CFD software packages are also complicated. An in depth breakdown of either the governing equations or the solution process utilized by FLUENT, the CFD software package utilized, is beyond the scope of this thesis. However, having a general understanding of the theory and solution algorithm is important for a several reasons, the first being to generate a proper physical model. For instance, when choosing the appropriate model simplifications, understanding the physics of the problem and how it relates to the governing equations is essential. Moreover, results generated using CFD are at best an approximation and at worst nonsense. Distinguishing between the two is often difficult, relying on user intuition. Therefore a good knowledge base of the theory will enhance the user intuition. The importance of understanding the solutions algorithm is because there are several variations available, of which some are more accurate than others when applied to certain problems. Thus, a grasp of the solution algorithm will help the user in choosing from the many available options.

For these reasons a brief overview of the governing equations and the solution process of FLUENT is given below. FLUENT itself utilizes the Finite Volume Method (FVM) to solve the governing equations and so a portion of this chapter is dedicated to an introduction to FVM. The final section deals with FLUENT program structure and certain aspects of the programs implementation.

Governing Equations

The governing equations of fluid dynamics are the fundamentals behind CFD. As mentioned earlier having a general understanding of the governing equation and of the numerical techniques used to solve them is necessary to successfully implement CFD software.

The philosophical procedure to generating the governing equations involves application of physical principles to that of a suitable fluid model, yielding mathematical equations. The three physical principles used are conservation of Mass and Energy as well as Newton's Second law. Two available fluid models are Finite Control Volume and Infinitesimal Fluid element. Figure 3-1 below shows a Finite Control volume. This

Figure 3-1: Finite Control Volume Fixed in Space. [Anderson, 5]

model is highlighted because it is the one chosen to generate the subsequent governing equations, and because it generates the integral form of the governing equations which are utilized in the FVM. Within the Finite volume element shown in figure 3-1, V is the

volume, S , is the surface and V is the velocity of the entire control volume (CV). Application of the Finite Control Volume involves integration over the entire CV.

Continuity Equations

For continuity, the physical premise is that mass is conserved, so that the net mass flow out of the CV plus the time rate of increase of mass inside the CV must equal zero. In mathematical form that statement becomes equation 2-1:

$$\frac{\partial}{\partial t} \iiint_V \rho dV + \oint_S \rho \mathbf{V} \cdot d\mathbf{S} = 0 \quad (2-1)$$

Note, in the continuity equation t represents time, ρ , the density of the fluid, and again V is the volume, S , is the surface and V is the velocity. The first term of equation 2-1 represents the time rate of increase of mass inside the CV and the second term represents the mass leaving through the surface, S .

Momentum Equations

The momentum equation is based on a general form of Newton's Second law, whose equation is:

$$\mathbf{F} = \frac{d}{dt}(m\mathbf{V}) \quad (2-2)$$

The variable F represents the net force exerted on the control volume, and that equals the time rate of change of momentum, where m is the mass and V is the velocity. Among forces acting on the CV include body forces, pressure forces and viscous forces. Pressure forces apply only to the surface of the control volume and so appear as a surface integral in the final momentum equation. On the other hand, body forces and viscous forces affect the entire CV and thus appear as volume integrals in the final equation. More specifically a

pressure force is $p dS$, where p is the pressure and dS is the area on which it acts. As for body forces are given by $\rho f dV$, where f represents the net body force per unit mass exerted in the fluid inside the CV. Finally F_{viscous} represents the total effect of the viscous forces.

On the other side of equation 2-2 is the time rate of change of momentum, which is equal to the time rate of momentum due to unsteady fluctuation of flow properties inside the CV plus the net flow of momentum of the CV. Finally equating the time rate of change of momentum to the sum of the forces acting on the CV leads to momentum equation, 2-3:

$$\frac{\partial}{\partial t} \iiint_V \rho \mathbf{V} dV + \iint_S (\rho \mathbf{V} \cdot d\mathbf{S}) \mathbf{V} = - \iint_S p d\mathbf{S} + \iiint_V \rho \mathbf{f} dV + \mathbf{F}_{\text{viscous}} \quad (2-3)$$

Energy Equations

The fundamental principle behind the energy equation is that energy cannot be created or destroyed, it can only change forms. Therefore the qualitative representation of the energy equation is given below:

$$\left[\begin{array}{c} \text{Rate of change of} \\ \text{Energy inside a CV} \end{array} \right] = [\text{Net heat flux}] + \left[\begin{array}{c} \text{Rate of work} \\ \text{done on CV} \end{array} \right]$$

Mathematically the rate of change of energy inside the CV is given by equation 2-4, below,

where $\left(e + \frac{V^2}{2} \right)$ is the total energy inside volume, V , and e is the internal energy.

$$\frac{\partial}{\partial t} \iiint_V \rho \left(e + \frac{V^2}{2} \right) dV + \iint_S \rho \left(e + \frac{V^2}{2} \right) \mathbf{V} \cdot d\mathbf{S} \quad (2-4)$$

The first term in equation 2-4 represents the time rate of change of total energy the CV due to transient variations of flow field variables, and the second is the net rate of flow of total energy across the control surface [Anderson, 5].

Next, the net heat flux is equal to:

$$\iiint_V \dot{q} \rho dV + \dot{Q}_{viscous} \quad (2-5)$$

In which case $\dot{q}$ is the volumetric rate of heat addition per unit volume and $\dot{Q}_{viscous}$ is the rate of heat addition to the CV due to viscous effects.

Finally the rate of work done encompasses the work done by the pressure forces, the body forces and the viscous effects. The three sources of work are shown below in equation 2-6, respectively.

$$-\iint_S p \mathbf{V} \cdot d\mathbf{S} + \iiint_V \rho (\mathbf{f} \cdot \mathbf{V}) dV + \dot{W}_{viscous} \quad (2-6)$$

The different components of energy together with the principle that energy is conserved generate the energy equation 2-7 given below.

$$\frac{\partial}{\partial t} \iiint_V \rho \left(e + \frac{\mathbf{V}^2}{2} \right) dV + \iint_S \rho \left(e + \frac{\mathbf{V}^2}{2} \right) \mathbf{V} \cdot d\mathbf{S} = \iiint_V \dot{q} \rho dV + \dot{Q}_{viscous} - \iint_S p \mathbf{V} \cdot d\mathbf{S} + \iiint_V \rho (\mathbf{f} \cdot \mathbf{V}) dV + \dot{W}_{viscous} \quad (2-7)$$

For a more in depth derivation of the governing equations see Anderson [5].

General Transport Equation

The governing equation given above can be written in a more general form, known as the general transport equation. First let ϕ represent a general variable per unit mass inside the control volume. Next define a general physical principle to govern the change of ϕ inside the CV, which is given below:

$$\left[\begin{array}{l} \text{Rate of} \\ \text{increase of } \phi \\ \text{inside a CV} \end{array} \right] + \left[\begin{array}{l} \text{Net rate of increase} \\ \text{of } \phi \text{ out of the CV} \\ \text{through the surface} \end{array} \right] = \left[\begin{array}{l} \text{Net rate of increase} \\ \text{of } \phi \text{ due diffusion} \\ \text{through CV} \end{array} \right] + \left[\begin{array}{l} \text{Net rate of creation} \\ \text{/destruction of } \phi \\ \text{due to sources} \end{array} \right]$$

The mathematical representation of the physical principle applied to a CV is given in equation 2-8, labeled the general transport equation.

$$\frac{d}{dt} \iiint_V \rho \phi dV + \iint_S \rho \phi \mathbf{V} \cdot d\mathbf{S} = \iint_S \Gamma \nabla \phi \cdot d\mathbf{S} + \iiint_V S_\phi dV \quad (2-8)$$

In equation 2-8, Γ is a diffusion coefficient and S_ϕ is a source term. For a more in-depth discussion and derivation of the general transport equation see Versteeg, [39].

The reason for the discussion of the general transport equation is because it is the best form of the governing equation when discussing the FVM. Using the general form entail the discussion of only one equation as appose to three.

Finite Volume Method

When it comes to CFD packages, they can be broken down into three key components, a pre-processor, a solver and a post-processor. The pre-processor handle the geometry setup and the subsequent grid generation. Once selection the physical or chemical process to be studied is done, one can proceed to defining the fluid properties and the appropriate boundary conditions. The solver, as the name suggest, is responsible for generation the solution. A solution may involve determining the pressure, velocity and temperature at nodal points throughout the computational domain. There are three main techniques available by which to generate the solution, Finite Difference Method (FDM), Finite Element Method (FEM) and Spectral Methods. A subset of FDM is the Finite Volume Method (FVM), and this method is that which FLUENT implements in its solution

process. The post-processor is a data visualization tool. Options available here include geometry and grid display, vector plots, contour plots, surface plots and particle tracking. Also important is view manipulation, such as zoom or rotation.

The first step in all finite volume methods is grid generation in which the domain is split into small control volumes. A 1D and 2D element used in the FVM are shown in figure 3-2 and 3-3 respectively.

Figure 3-2: 1D Finite Control Volume.

Figure 3-3: 2D Finite Control Volume. [Versteeg, 39]

The center of the control volume is given by nodal point P. Nodal points W and E are the center points of the control volumes on the west and east side of the control volume about

point P, respectively. Similarly N and S are the northern and southern center points of control volumes in a 2D scheme. On the surface adjoining cell volumes are points labeled by the corresponding lower case letter. For example the surface joining cell W and cell P is w. The grid size, Δx and Δy are width and height of the control volume as shown in the figure 3-3. Another labeling convention shown figure 3-2 is the use of δ to represent the distance between points, with its subscripts denoting which points. For instance, $\delta_{x_{wp}}$, represents the distance between the W and P nodal points, or $\delta_{x_{pe}}$, which represents the distance between P and e.

The next step is discretization of the governing equation. Discretization involves integrating over the control volumes to create discrete equations, valid for the nodal point of the grid. To illustrate the discretization process, take for example the 1D steady state diffusion of ϕ in the transport equation given below in equation 2-9.

$$\iiint_V \frac{d}{dx} \left(\Gamma \frac{d}{dx} \right) dV + \iiint_S S_\phi dV = 0 \quad (2-9)$$

Being steady state eliminates the time dependent term of transport equation and by stating only diffusion eliminates the convective term, $\iint_S \rho \phi \mathbf{V} \cdot d\mathbf{S}$. Equation 2-9 is similar to that of a 1-D heat transfer.

Evaluate the integrals of equation 2-9 on the surface points of a 1-D control volume similar to that of figure 3-2 one yields equation 2-10.

$$\left(\Gamma A \frac{d\phi}{dx} \right)_e - \left(\Gamma A \frac{d\phi}{dx} \right)_w + \bar{S} \Delta V = 0 \quad (2-10)$$

In equation 2-10, A, represents the area of the corresponding cell side and $\bar{S}$ is an approximation of the source term in the CV. Then one can approximate the value at the

control volume surface, e and w, using the data at the cell center for adjacent cells, as shown in equation 2-11 and 2-12.

$$\left(\Gamma A \frac{d\phi}{dx} \right)_e = \Gamma_e A_e \left(\frac{\phi_E - \phi_P}{\delta_{PE}} \right) \quad (2-11)$$

$$\left(\Gamma A \frac{d\phi}{dx} \right)_w = \Gamma_w A_w \left(\frac{\phi_P - \phi_W}{\delta_{WP}} \right) \quad (2-12)$$

As is often the case the source term source term may be a function of the independent variable, ϕ , so the source term can be approximated as:

$$\bar{S} \Delta V = S_u + S_p \phi_p \quad (2-13)$$

Next sub in equation 2-11 through 2-13 into 2-10 and rearrange to get:

$$\left(\frac{\Gamma_e}{\delta x_{PE}} A_e + \frac{\Gamma_w}{\delta x_{WP}} A_w - S_p \right) \phi_p = \left(\frac{\Gamma_w}{\delta x_{WP}} \right) \phi_W + \left(\frac{\Gamma_e}{\delta x_{PE}} \right) \phi_E + S_u \quad (2-14)$$

All terms within brackets and S_u in equation 2-14 are known, and so is a linear equation for a general CV. Therefore one can generate a series of linear equations for a given grid and proceed to solving then given the appropriate boundary conditions.

In regards to treatment of nonlinear terms in the governing equations there are a couple approaches as how to linearize them. One is done by lagging the coefficients. To best illustrate the concept take equation 2-15, whose linearized form using lagging coefficients is 2-16.

$$S = 4 - 5T^3 \quad (2-15)$$

$$S = 4 - 5(T^n)^2 T^{n+1} \quad (2-16)$$

In equation 2-15 and 2-16, S is some arbitrary source term which is a function a variable in the governing equation, such as temperature. Here the cubic non linear temperature term is linearized taking some known information of the previous time step, denoted by 'n', splits

the nonlinear term such that only one variable of the current time step, 'n+1' remains; hence the label lagging. Another technique is Newton Linearization, which states:

$$F^{n+1} = F^n + \frac{\partial F}{\partial Q} \Delta Q \quad (2-17)$$

where F is a function of an arbitrary variable, Q. Given the same example of equation 2-15, the Newton linearized version is shown below:

$$S = 4 - 5(T^n)^3 - 15(T^n)(T^{n+1} - T^n) \quad (2-18)$$

Again notice that only one term of the current time step 'n+1' is remaining.

Solving the governing equation may appear simple up to this point, but there is one major complicating issue. The problem arises due to the existence of both convective and diffusive terms in the governing equation. The influence on a given point due to convective terms in the governing equation is dependent on the flow direction while no so for diffusion terms. Therefore a central differencing approximation for data at a control volume's edge is a good representation for diffusive terms but not for convective because it does not consider the flow direction. To address this issue a term, Peclet Number, is defined which measures the ratio of diffusion to convection. Equation 2-25 shows Pechel Number mathematical definition.

$$Pe = \frac{\rho V L}{\Gamma} \quad (2-25)$$

If $Pe \gg 1$ convection dominates and if $Pe=0$ only diffusion exists. Using Pe as a guide several scheme were devised to improve independent variable's approximation. For instance the Upwinding scheme is gear towards convection dominated flows. This scheme uses one side difference approximation whose direction is opposite to that of the flow direction. Hence only upwind nodes will influence the approximation. The Hybrid scheme is based on

a combination of the central differencing and upwinding scheme. Other schemes include Power-law and Quick.

Now to solve the governing for the desired field variables like velocity and pressure requires the tools given above as well as an iterative procedure. One such iterative approach is the SIMPLE algorithm. Start the process by guessing the initial pressure field, p^* . Next, use the momentum equation to solve the resulting u^* , and v^* . In a converged solution the pressure field used in the momentum equation will generate velocity values that satisfy the continuity equation. Therefore using the continuity equation it is possible to generate a pressure correction formula that produces p' , a correction pressure value that adjusts the initial pressure estimate. Hence the next step is correction to the initial pressure guess. Subsequently the following equation is used to correct the velocity values developed in the second step:

$$u_e = u_e^* + d_e(p'_P - p'_E) \quad (2-26)$$

where $d_e = A_e / a_e$

Equation 2-26 is for one side of a control volume, similar equation exist for the other sides. Furthermore this equation is the main assumption of the SIMPLE algorithm, and is derived from the discretized momentum equation with a logical simplification relating the fact that the correction values drop to zero upon conversion. At this point one can solve for other transport variables such as temperature. Quick test for convergence and if no the corrected values for pressure and velocity not become the new guess values for the next iteration. There are variations of this algorithm, namely SIMPLER, SIMPLEC and PISO, which alter a few steps but follow a similar procedure. Note, the iterative algorithms here are for incompressible flow scenarios.

For more on the Finite Volume Method see Versteeg, [39].

FLUENT Theory and Application

FLUENT is design to simulate a wide variety of different flows and heat transfer problems. The program structure is laid out in figure 3-4.

Figure 3-4: FLUENT Program Structure [FLUEN, 12]

In essence FLUENT is only a solver, it requires an external program to generate the geometry and the corresponding grid. GAMBIT is one such program that accompanies the FLUENT software package. Alternatively other CAD/CAE programs such as ANSYS can be used to generate the geometry and grid, and then be imported into FLUENT. However GAMBIT was the program used to generate the geometry and grid in all the valve cases. A supplementary tool available in the FLUENT software package is TGRID which can further manipulate the grid to be solved. Within FLUENT, the solver, the user imports the mesh, sets the physical model, the boundary conditions and material properties followed by calculations and postprocessing.

Implementing FLUENT requires four main steps. The first step is to define the modeling goals. The second step is to set the computational model, in which one creates the geometry of the system, generates a grid and sets the boundary conditions. The third step involves the choosing the appropriate the physical model, aimed at proper representation of the physics behind the problem. The final step is the determination of the solution procedure. At this point the solution scheme and parameters are set to best suit the problem at hand, in an attempt to avoid convergence issues and generate the solution as efficiently as possible.

Boundary Conditions

Boundary Conditions are necessary component of a CFD solution process, and there are a number of different types; each having its own numerical implications. The boundary types available in FLUENT are classified as follows [FLUENT, 12]:

- Flow inlet and exit boundaries: pressure inlet, velocity inlet, mass flow inlet, inlet vent, intake fan, pressure outlet, pressure far-field, outflow, outlet vent, exhaust fan
- Wall, repeating, and pole boundaries: wall, symmetry, periodic, axis
- Internal cell zones: fluid, solid (porous is a type of fluid zone)
- Internal face boundaries: fan, radiator, porous jump, wall, interior

The role of a Boundary Condition is to provide the necessary information to make the solution process possible.

When dealing with thixomolding the relevant inlets are pressure inlets, a velocity inlets and a mass flow inlets. The information available for a pressure inlet is obviously the pressure, and is used when the mass flow rate or the velocity of the incoming flow is unknown. Similarly for the other two inlets the information available at the inlet is velocity and mass flow respectfully.

Essentially there is a relationship between velocity, pressure and mass flow, so that if one is fixed in the iteration process the others are allowed to fluctuate to maintain the applied value. “FLUENT then uses the boundary condition inputs to compute the mass flow into the domain through the inlet and also to compute the fluxes of momentum, energy, and species through the inlet.” [FLUENT, 12].

Flow outlets of particular interest to thixomolding include the pressure outlet and the outflow condition. Again a pressure outlet is used when the pressure at the outlet is known. Here the static pressure is specified at the outlet, while all other conditions, such as velocity, are extrapolated from the conditions in the interior domain. Utilizing a pressure outlet may induce a backflow condition, wherein the state of the back flowing must be specified such that convergence may continue. An outflow condition is used when the details, that is, variables like pressure and velocity at the outlet are unknown. In the case of an outflow outlet the diffusion flux for all variables is assumed to be zero. In other words the flow is assumed fully developed, such that it will have no effect on upstream conditions. Variable at the outflow are extrapolated from the interior, keeping in mind the flow is fully developed.

Other important boundary conditions include walls, symmetry and axis. A wall is the boundary between a solid surface and the fluid. At such a juncture with viscous flow a no slip condition is applied wherein the velocity of the fluid is set to that of the wall. Symmetry is used in the case when the geometry is such that the flow exhibits mirrors itself about the symmetry surface. This boundary condition is useful to reduce the size of the computational domain. With symmetry one assumes zero flux for all quantities and zero normal velocity across this surface. The axis boundary condition is used in conjunction to axisymmetric problems. It denotes the centerline of the geometry. The physical values on the centerline are extrapolated from the adjacent cell.

Physical Properties

Physical Properties describe the physical model used in the solution process. They describe the properties of the fluid and how these properties are approximated. Some physical properties include density, viscosity, heat capacity, thermal conductivity, standard state enthalpies and kinetic theory parameters.

Of the physical properties, those most relevant to a thixomolding CFD model are density, viscosity and thermal conductivity. The fluid, Magnesium alloy, is incompressible, and so the density is set to as a constant. In regards to viscosity, FLUENT allows for a variety of options. It can be set to constant, a temperature dependent function, or to Non Newtonian, all of which are viable options for the proposed model. As for thermal conductivity, it can be set to constant or a temperature dependent function. Knowing the options available for the physical properties is important to ensure the most accurate physical modeling.

Dynamic Mesh

Dynamic Mesh is used to model flow where the domain is changing shape. Therefore motion is specified on a surface, and internal mesh is forced to change to accommodate the moving surface. The motion itself is set about the center of gravity and follows solid-body-kinematics [FLUENT, 12]. To start FLUENT requires an initial volume and mesh, which will subsequently be altered due to the applied motion. Updating of the mesh is handled automatically by FLUENT, with some guidance parameters inputted by the user. Both moving and non-moving surfaces must be specified, with options for a surface being, moving, stationary or deforming.

Obviously a Dynamic mesh is only possible with unsteady flow being that it is time dependent. The deforming domain will obviously have an affect on the general governing equation, and so equation 2-30 shows the revised general conservation equation.

$$\frac{d}{dt} \iiint_V \rho \phi dV + \iint_S \rho \phi (\mathbf{V} - \mathbf{V}_g) \cdot d\mathbf{S} = \iint_S \Gamma \nabla \phi \cdot d\mathbf{S} + \iiint_V S_\phi dV \quad (2-30)$$

In that equation, 2-30, $\mathbf{V}_g$ stands for the grid velocity. Furthermore the volume is now changing and thus must be included in the time derivative in a manner shown in equation 2-31.

$$\frac{d}{dt} \int_V \rho \phi dV = \frac{(\rho \phi V)^{n+1} - (\rho \phi V)^n}{\Delta t} \quad (2-31)$$

Equation 2-31 assumes a first order backward difference approximation for the time derivative. A formula is needed to compute the volume, V , at time interval $n+1$, given by equation 2-32 and 2-33.

$$V^{n+1} = V^n + \frac{dV}{dt} \Delta t \quad (2-32)$$

$$\text{where } \frac{dV}{dt} = \iint_S \mathbf{V}_g \cdot d\mathbf{S} = \sum_j^{n_f} \mathbf{V}_{g,j} \cdot \bar{\mathbf{A}}_j \quad (2-33)$$

Equations 2-30 through 2-33 give a brief description of how continuity is maintained given that the boundary is moving.

In regards as to how exactly the mesh is updated, there are three available options, spring-based smoothing, dynamic layering and local remeshing. In spring-based smoothing the layers of cells act like a series of connected springs whose stiffness is set by the user. A displacement of a boundary is converted to a force based on Hooke's law for springs. The series of spring distribute the force throughout layers causing a smooth distribution of the displacement. Therefore all of the elements adjust slightly to accommodate the applied

displacement. Figure 3-5 shows spring-based smoothing of a cylinder which is being compressed.

Figure 3-5: Illustration of Spring-Base smoothing. [FLUENT, 12]

The next remeshing option is dynamic layering which requires hexahedral or wedge elements to be applicable. Here only one layer of elements is affected by the motion and it either collapses or splits to accommodate the moving surface. To do so the user sets an ideal cell height, h_{ideal} , and a split factor, α_s . When the condition of equation 2-34 is met the layer of elements attached to the moving surface splits.

$$h_{cell} > (1 + \alpha_s)h_{ideal} \quad (2-34)$$

The splitting of the layer can be done by cutting the deformed layer in half or by creating one layer with ideal height and one with height the remain length. Collapse of a layer is done if the condition of equation 2-35 is met.

$$h_{cell} < \alpha_s h_{ideal} \quad (2-35)$$

In the event of collapse the adjacent layer absorbs the height of the deleted layer.

The final remeshing option available is local remeshing and it is designed for triangular or tetrahedral elements. The main ideal behind this technique is to local remesh elements which become distort due to the motion of the grid. There are three criteria that constitute a distorted element and if any of the three is met the element is marked for remeshing. The first being that a cell must remain below a maximum cell volume, secondly it must remain above a minimum cell volume and lastly the skewness must stay below a set value. These three distortion limits are set by the user.

The various remeshing option can be used in conjunction with each other such that a wide variety of domain motions can be modeled.

Modeling Solidification and Melting

The solidification and melting option in FLUENT is used in problems where conditions are such the fluid is experiencing solidification and or melting. FLUENT is not limited to a fixed value of melting temperature; it has the capabilities to model fluids which have a melting temperature range. This capability is especially important when modeling a thixomolding process because the molten material is by definition in the semi-solid state during injection, that is the melt temperature falls on the melting temperature range. The program does not, however, have the means of explicitly track the melt. Instead the mushy zones are treated as a porous solid, with a porosity value equal to liquid fraction. Liquid Fraction, β , is a parameter that measures the ratio of liquid in a cell. When a cell completely solidifies the porosity is zero and so the velocity in that that cell also becomes zero. Solid zones are modeled as sinks to generate the appropriate pressure drop.

When activating the solidification and melting option in FLUENT, one is limited to incompressible flow and the segregated solver [FLUENT, 12]. Also additional material

properties are required, such as the melting temperature range, given by a T_{solidus} (solidification temperature), T_{liquidus} (melting temperature), Latent Heat and C_p .

The influence of the solidification and melting aspect of the model reaches the energy equation via enthalpy, and the momentum equation by means of the sink terms. Enthalpy in FLUENT is calculated by adding the sensible enthalpy, h , to the latent heat, ΔH , and shown in equation 2-36.

$$H = h + \Delta H \quad (2-36)$$

When solidification and melting is enabled, the latent heat of equation 2-36 is adjusted based on the liquid fraction value of the cell, shown in equation 2-37.

$$\Delta H = \beta L \quad (2-37)$$

Here L is the Latent Heat of the material and ΔH is the corrected latent heat. As for the liquid fraction, β , it is calculated using the lever rule and the temperature of the cell, T , shown in equation 2-38.

$$\beta = \frac{T - T_{\text{Solidus}}}{T_{\text{Liquidus}} - T_{\text{Solidus}}} \quad \text{if } T_{\text{Solidus}} < T < T_{\text{Liquidus}} \quad (2-38)$$

As mentioned, the liquid fraction appears in the momentum equation in the form of a sink and the formula for set sink is given in equation 2-39.

$$S = \frac{(1 - \beta)^2}{(\beta^2 + \epsilon)} A_{\text{mush}} (V - V_p) \quad (2-39)$$

The ϵ variable is a small arbitrary number used to prevent division by zero, A_{mush} is a mushy zone damping term, and V_p is the velocity of the solidus material if being pulled out of the domain. In all, the implementation of the solidification and melting option to the modeling to that of the standard solver is quite simple, however, it does increase the computation time.

User Defined Files

“A user-defined function, or UDF, is a function that set by the user and can be dynamically loaded with the FLUENT solver to enhance the standard features of the code.” [FLUENT, 12]. In other words FLUENT enables the user, with some restriction, to improve or expand the capabilities of FLUENT itself. For instance a UDF can be used to apply an alternative physical model, such as an empirical model for viscosity of a non-Newtonian fluid. UDF's allow modification of boundary conditions, material properties and source terms; at any given time in the solution process. Furthermore, UDF's can access solver data in its calculations, allowing access to such data velocity values, pressure values and temperature values. In regards to the calling sequence in FLUENT, a UDF may be called upon at the initialization stage, on demand, and at the end of an iteration. Figure 3-6 illustrates the options available in regards to calling UDF.

These files are written in a C programming language, and along with the functions of that language, FLUENT provides its own set of predefined macros and function which allow access to solver data. The files can be compiled internally by FLUENT, known as interpreted compiling, or externally, known as compiled functions. The internal process for interpreted compiling make it architecture independent allow for easy case transfer between computers. However, coupled with the internal process is a performance penalty, so that external compiling may be the best choice for computationally expensive models.

Figure 3-6: Calling sequence diagram for a UDF [FLUENT, 12].

Chapter 4 Valve Modeling Procedure

The first step in the modeling process is to set up the geometry to be used. The valve design is simplified to the point that it still remains true to the actual component but is free of details, to avoid complications in the CFD modeling. For example, there are few O rings seals which are part of the valve design; however they are not included in the CFD model. These O rings are small and difficult to include in a CFD model; the mesh would have to be extremely fine in these areas and yet have little influence on the overall forces acting on the valve. Hence they were not incorporated.

The next step in the modeling process is to generate a mesh which will accommodate the moving components, that is, a grid subject to adaptation while still maintaining convergence. Once a suitable mesh is created the next logical set is to feed a solver with a slue of input parameters and boundary conditions. The solution can then be post-processed and examined. All of which is typical CFD solution process.

Valve Geometry

As stated earlier, to begin modeling, the valve geometry was established. A three dimensional (3D) rendering of valve assembly is given in figure 4-1; along with the labels of various components. The main parts of the valve are the Ring and Valve Body. The valve itself is attached to the Screw Shaft and housed by the Barrel, also known as the housing cylinder. Dimensionally the valve is relatively small. The inner radius of the barrel is (35mm), and the valve length is on the order of twice the radius.

Figure 4-1 - Valve Assembly

The valve is further broken down in figure 4-2 in which the valve Body and Ring are shown separately. Furthermore the Ring is sectioned for a better view of the inner structure.

Figure 4-2 - Valve Components. The Valve Body is on the Left and Ring on the right.

In figure 4-2 the features described in an earlier chapter are more easily observable. On the valve body the four flutes are visible, that is, the grooves on the stud (valve tip) which allows

flow passage during the open configuration. Moreover the rear seat of the valve is characterized by the sharp increase in shaft radius towards the back of the valve. The angle of that sharp increase corresponds to the angle at the back of the ring component, such that in the closed valve configuration these two surfaces in contact provide the seal. From the fully open to the closed state the Ring travel approximately (4mm); a size small enough to achieve the rapid operations speeds required.

Geometric Simplifications

The Nozzle shown in figure 4-1 is mainly for illustration sake and was not included in the model. The reason for its exclusion is simply to reduce the size of the model so that the focus of the mesh would be on the valve rather than the downstream effects of the nozzle. This simplification is easily justifiable because at the point of closure the valve is at its farthest distance from the nozzle. Also results will show that the downstream effects can be modeled as a slight back pressure condition at the outlet, validating the omission of the nozzle.

Another geometric simplification which may require justification is the exclusion of the gap between the ring and the barrel. Two conditions must be met for this assumption to be valid; firstly the mass flow through the gap must be negligible and secondly the viscous forces generated between the ring and barrel must also be insignificant. Therefore to justify the simplification a case which includes the gap is required with the main focus on measuring the relative strength in the two areas mentioned.

A course mesh of the 3D valve can easily surpass one million elements, which means generating an unsteady solution requires a great deal of time. Compounding the mesh size issue is the fact that FLUENT has a limitation in which symmetry cannot be used with

the dynamic mesh option [FLUENT, 12]. This option is required for all cases to account for the motion of the valve. Being that an extensive amount of control variables are being explored and a great deal of model validation is required all leads to the fact that many CFD case runs are necessary. Therefore in an effort to reduce the computation time some exploration of a 2D axisymmetric model was done. The 2D model generation process is illustrated in figure 4-3.

Figure 4-3 - Generation of the 2D Axisymmetric Model.

To make the 2D axisymmetric model useful, a few conditions must be met. First off the computational benefits must be significant, which they are. The Axisymmetric model cut down the computation time from days to hours. A second condition is that the results generated must be comparable an area addressed in chapter 4.

The main idea behind the 2D axisymmetric model was that of a supplementary tool used to guide the more computationally expensive 3D model. For example the 2D

axisymmetric model can be used to optimize the convergence rate using a trial and error method within a few hours such that the 3D model, which takes days to solve, may be much more efficient. However, should the correlation between models be good, meaningful results may be extrapolated from the 2D axisymmetric model. In the end both the 3D and 2D axisymmetric model will be used carefully in conjunction with each other. A side benefit to the 2D axisymmetric model is that it will illustrate the influence of the valve stud on the design.

Meshing Procedure

Given that the geometry is set, the next point of interest is with respect to mesh generation. The decision was made to use an unstructured mesh, utilizing triangular elements, for three reasons. The first being that generating a smooth quadrilateral mesh is extremely difficult given the complexity geometry of the valve. The mesh generation was accomplished using a program called GAMBIT, commonly used in conjunction with the CFD program FLUENT. With the capability of GAMBIT creating a structured mesh, especially when considering the curved flutes on the stud, is time consuming and runs into skewness issues. In short an unstructured mesh is easier to generate. The second reason is that an unstructured mesh will provide that same solution once converged. Finally, and perhaps the most important reason, is that an unstructured mesh couples best with the motion of the valve when considering the capabilities of FLUENT. To create a structured mesh that could contend with the opposing motion of the valve components requires the creation of many interior zones, which greatly increase the complexity of the model.

To determine the best suitable mesh size required research into the matter through essentially a trial and error method. Also a mesh analysis is necessary because there are no

experimental results available to justify results. Therefore the first set of cases run deals with determining the results convergence as the element size decreases. One can then establish a suitable element size that is computationally viable and within acceptable error limits. This area of research is well suited to the 2D axisymmetric model because the results themselves are not important, but their convergence in relation to element size is.

The element size remains essentially constant throughout the fluid volume mainly to cater to the remeshing algorithm of FLUENT. In the 2D axisymmetric model a triangular element was used throughout the entire fluid domain. However the 3D model contains a portion of the barrel downstream of the valve which consists of quadrilateral elements and the valve itself is encased in tetrahedral elements. Figure 4-4 illustrates a plane cutout of the mesh, and it clearly shows the transition from tetrahedral to quadrilateral elements.

Figure 4-4 - Plane Cutout of 3D Mesh.

The valve assembly moves at a relatively fast speed, and thus a long barrel section is required to accommodate the forward valve movement. Nonetheless using tetrahedral elements to fill the empty barrel section is inefficient. When the geometry is a simple cylinder, as it is with the barrel shape downstream of the valve, a quadrilateral mesh and its accompanying

remeshing scheme are a better choice. A grid interface marks the transition from tetrahedral to quadrilateral elements. This interface is essentially an interior face which travels at the same speed as the valve body. Therefore the grid interface will always be a set distance downstream of the valve tip and because it is an interior zone it has no affect on the solution. Moreover this allows the tetrahedral mesh to encompass the region with highest influence from the valve, while leaving the quadrilateral mesh to handle the section where little is going on. In the end the model becomes slightly more complicated, but more importantly is less computationally expensive.

Mesh Motion

The motion of the valve body is a known variable, set by either a constant hydraulic force on the screw shaft or a set velocity on the shaft. However the ring is free to move based on the pressure gradients created by the valve body's motion and hampered by viscous forces. The progression of the mesh is given in figure 4-5a through 4-5e, which are a set of frames taken at different points in the solution; focusing on the rear of the ring and the seat of the valve body. The frames show that as the motion progresses the remeshed elements tend to be smaller in size, a phenomenon purposely done to ensure the skewness of the elements remains under acceptable limits as the gap between becomes increasingly smaller. It is also intended to keep as many elements in the gap for as long as possible while not dragging the solution computationally. However, as a result of that intention, a small amount of clustering appears in the mesh in the region surrounding the contact surface. The clustering is unavoidable due and of little significance to the final solution.

Grid (Time=0.0000e+00)

FLUENT 6.1 (axi, dp, segregated, dynamesh, lam, unsteady)

Apr 28, 2005

Figure 4-5a: Frame of Mesh Progression through time ($t=0$ sec).

Grid (Time=5.0000e-04)

FLUENT 6.1 (axi, dp, segregated, dynamesh, lam, unsteady)

Apr 28, 2005

Figure 4-5b: Frame at $t=5 \times 10^{-4}$ sec.

Grid (Time=1.0000e-03) FLUENT 6.1 (axi, dp, segregated, dynamesh, lam, unsteady) Apr 28, 2005

Figure 4-5c: Frame at $t=1 \times 10^{-3}$ sec.

Grid (Time=1.5000e-03) FLUENT 6.1 (axi, dp, segregated, dynamesh, lam, unsteady) Apr 28, 2005

Figure 4-5d: Frame at $t=1.5 \times 10^{-3}$ sec.

Grid (Time=2.0000e-03)

FLUENT 6.1 (axi, dp, segregated, dynamesh, lam, unsteady)

Apr 28, 2005

Figure 4-5e: Frame at $t=2 \times 10^{-3}$ sec.

The model solution is stopped once the skewness exceeds set limits or if a negative cell volume is created. The mesh motion process is the same for the 3D model, except the fact the viewing the mesh progression is not possible other than monitoring the maximum cell skewness.

Another limiting factor on the element size deals with the negative cell volume situation. The valve operation occurs at a relatively high velocity and couple with small geometry size enforces certain limits on the time step or the element size. It's the balancing act of all CFD models. After every time step the boundary nodes of both the ring and valve body are shift to simulate the motion of the valve. If the velocity is fast enough the cells do not just compress, but actually invert, creating a negative cell volume. Such a case is a fatal error in CFD code. There are two ways to solve this problem; one is to decrease the time step such that the distance traveled by the same velocity is smaller. The second is to increase the element size such that it can accommodate a larger node shift without inverting. In

short, it's another factor to consider, one that if neglected would lead to premature solution conclusion.

Imposing the motion of the valve is governed by external user defined files (UDF). One UDF was used to set the velocity of the valve body. Another was used to access solver data and compute the force on the ring. The same file then calculates the resulting velocity and imposes it on the ring. A copy of both files is given in the Appendix labeled UDFs.

The valve body file works on a simple principle. After every time step the FLUENT case consults the file for the velocity of certain boundary nodes. The link between the file and the boundary is set during the case setup by the user. For the valve body, the boundary is set to rigid body motion, and other dynamic zone options include deforming and stationary boundaries. Within the file can be any polynomial that considers the time as a variable can be used, creating any desired velocity profile. In the file given in the appendix the velocity of the body is desired to be constant at (2.5 m/s). Setting the velocity of the valve body directly to that value at the start of the solution induces numerical instability, due to the step function nature of the velocity profile. It is customary in CFD solutions to have a ramp-up progression of the velocity, which means a small period of gradual acceleration until the desired velocity is reached. Utilizing, more accurately resembles the actual process because step functions are ideal and during the real process a small acceleration period most definitely occurs. Justification of the ramp-up function is given in the up coming results.

As for the governing file used in conjunction with the ring, it is more complicated. The file uses the basic principle of Newton's Second Law:

$$F_{\text{net}} = ma \quad (3-1)$$

The forces on the boundary faces are summed to calculate the net force on the ring. The mass is known, and so an acceleration value for the ring is easily calculated. This

acceleration is assumed constant over the small time step and can be used to find the change in velocity using the following basic motion equation:

$$\Delta V = a\Delta t \quad (3-2)$$

The file stores the previous time step value for ring velocity, adds it to the calculated change in velocity and exports that as the new velocity. Note the file exports the ring velocity and the results distance travel is calculated internally by FLUENT itself. Initially the ring starts at rest.

Case Variations Modeled

Many cases are required in an in-depth analysis of the valve in question. The plan is to split the total number of cases into three main categories; first set attempt to validate the model, the second aim to gain a knowledge base of the valve and the final set addresses possible design alterations.

Under the scope of the validation section is a steady solution in which the motion of the valve is fixed. Instead the fluid is set in motion around the valve. The idea here is to generate a fine mesh that remains unchanged avoiding the mesh degradation that comes with remeshing. One can then test the benefits of structured or unstructured meshes, the relative strengths of the pressure forces in comparison to the viscous forces, and incorporate the gap between the ring and the barrel to validate its omission in the unsteady solution. Next a slue of baseline tests are run with various element sizes to help justify the grids of the following cases. Also they provide a baseline for comparison to be used against other cases. The next logical set of cases that test the effect of a decreasing time step size on the model output to determine the ideal value. Following these cases, one should explore the effect of the ramp-up feature in the Valve Motion UDF on the output results. The final area of validation

should explore the correlation strength between the 2D axisymmetric model to the full 3D version.

The extent of the knowledge base category of results basically entails the variation of certain parameters and monitoring their effects. One such case would entail altering the nozzle back pressure and examining the effect on the ring velocity profile. Going back to the main purpose, results pertaining to the thixotropic properties of the material should be tackled here. Therefore cases examining the effect of changing the material from an average plastic to that of molten magnesium are a good area to explore. Furthermore one should research the effect of the semi solid material properties, by allowing solidification and melting of the fluid based on the temperature contours.

The final class of results delves into altering the valve design. A set of cases would deal with altering the geometry, which would involve altering the incoming and outgoing angles on the ring in an attempt to determine its effects on the output. To do so would entail altering the valve body as well, such that the seat and stud have the same angles as their corresponding ring surface in order to maintain the seal when in contact.

Flow Material Properties

For the many cases the properties of the fluid are common. For those utilizing the magnesium allow, table 3.1 lists the values can be used. These values are all assumed constant throughout the solution process.

Density	1830 kg/m ³ (at 20 °C)
Solidus Temperature	470 °C
Liquidus Temperature	595 °C
Kinematic viscosity	0.0012 m ² /s (at 590 °C)

Specific Heat	1014 J/kgK (at 20°C)
Thermal conductivity	72 W/mK (at 20°C)
Latent heat	3.73×10^5 J/kg

Table 4-1: Properties of Magnesium Alloy AZ91D

For a case with which to compare the magnesium alloy results to those of an average plastic involves using the properties of table 3.2. Many of the plastic polymers used in injection molding were considered and the properties listed in table 3.2 are an average of the various plastics.

Density	1000 kg/m ³ (at 20°C)
Kinematic viscosity	$1e-6$ m ² /s

Table 4-2: Properties used to simulate various Plastic Polymers

Chapter 5 Results

Model Validation

The results here are geared towards model validation. In doing so three areas will be addressed, one being the simplifications to the geometry, the second is to determine the optimal time step size and the finally to establish a suitable mesh size.

Steady State Analysis

Under the title of steady state analysis lies a case in which the valve is fixed in the open configuration and the fluid is set in motion at (1 m/s) around it. In other words upstream boundary is set as a velocity inlet with incoming flow of (1 m/s) and the downstream counterpart is set to outflow. The barrel pressure, or internal pressure was set to (30 MPa), a common injection pressure.

The model is set as 2D axisymmetric and the geometric configuration is shown in Figure 5-1. The yellow edge is the axis of symmetry, the blue edge corresponds to the velocity inlet and the red is the outflow. Also the figure shows key features which were included, namely the gap between the Ring and the barrel and the valve stud. Here the stud accelerates the flow as it approaches the gap, hence inducing the most flow into the gap. The flutes, or gates, on the stud were not included because they would not allow for a 2D axisymmetric model. These flutes would take away from the flow velocities near the gap, so that without them the leakage through the gap would be at its worst. Therefore if the leakage is negligible here, then with the gates, it is even less of a concern.

Figure 5-1: Valve Geometry Including Gap between Ring and Barrel. Top illustrates the entire model, and below is a closer view of the highlighted area.

With regards to the meshing of the fluid domain two approaches were used, one utilizing quadrilateral elements and the other with triangular elements, of which a portion is shown in Figure 5-2 and 5-3, respectively.

Figure 5-2: Quadrilateral Mesh

Figure 5-3: Triangular Mesh

As touched upon earlier the purpose of testing both mesh types is to evaluate the accuracy of the results, as well as comparing the rate and ease of convergence.

The simplest methods to determine the precision of the model is to examine the mass flow results. The flow is incompressible internal flow, such that a quasi-one-dimensional continuity equation, equation 4-1, can be used to ascertain the flow velocity at the outlet.

$$A_1 V_1 = A_2 V_2 \quad (4-1)$$

The areas are known, the input velocity is set to (1 m/s), thus the outflow velocity should be (3.769 m/s). Both meshes converged quickly to the calculated value with (3.7696 m/s) and (3.7675 m/s) for the quadrilateral and triangular meshes respectively. Figure 5-4 shows the convergence of the outflow velocity for the triangular mesh; where in the quadrilateral counterpart produces a nearly identical plot.

Figure 5-4: Outflow Velocity

The mass flow parameter verifies that the continuity equation is converging in the model, but at the same time gives no insight into the validity of other parameters such as pressure and fluid velocity about the valve itself. In an attempt to verify the convergence of such contours, one can monitor the force on certain parts. The force acting on a component is directly coupled to both the velocity of the fluid and the pressure acting on various walls. Therefore, if the net force on a component converges then so must the velocity and pressure contours throughout the fluid field. Figure 5-5 outlines the convergence of the net force acting on the ring component of the valve assembly, for both meshes. In figure 5-5, the quadrilateral mesh is shown to take about twice as many iterations to converge; however, per iteration, less time is required. In the end, convergence takes relatively the same amount of time for both meshes. Final convergence of the drag acting on the ring for the quadrilateral and triangular meshes are (-358.773 N) and (-378.834 N) respectively. The negative value is consistent with the direction of

Figure 5-5: Convergence of Force on Ring

flow. Furthermore, the variation between cases is approximately 5.5%, an acceptable value; however, it does point out an area of concern in an unsteady solution. Is it a compounding error source that grows from one time step to the next, and if so does a smaller time step curb its influence? This issue will be addressed shortly in an upcoming section and shown to be insignificant.

An interesting revelation encountered in both of the steady state cases is that the viscous forces are slightly less than one Newton. Therefore, the viscous forces are insignificant when compared to the large internal pressure forces generated by the valve movement in terms of its contribution to the ring motion. This validates the omission of viscous forces in the valve UDF. As mentioned earlier, the valve UDF sums takes the force value generated by FLUENT and uses that to set the ring velocity for the following time step. The force value itself is calculated by summing the pressure values of element edges attached to the boundary of the component in question. The fact that the viscosity is insignificant to the generated motion does not mean that the viscosity itself is insignificant.

The high viscosity ensures the flow remains laminar and thus the model setup remains valid. It also provides numerical damping which enables the convergence of results in every time step, a fact that is apparent in an upcoming section.

Upon closer examination of the pressure and velocity contours plots, they appear logical given the flow conditions. Take for instance figure 5-6 which gives an illustration of the pressure contours over the entire model. The dominant feature of figure 5-6 is the increased pressure in front of the valve, which is simply attributed to the constricting area.

Figure 5-6: Pressure Contours

As the flow encounters the stud, the area is decreasing, thus the flow is accelerated and consequently the pressure builds up. Zooming into the ninety degree corner, more features of the pressure field become visible, as seen in figure 5-7. Here, results are similar to the classic backward facing step of CFD. Immediately following the corner, a low pressure

Figure 5-7: Closer Examination of Corner Pressure Contours

point is visible which causes the flow to turn. Also the fluid curls about the low pressure point. Figure 5-8 shows a vector plot of the same corner, pointing out the fluid curl just mentioned.

Figure 5-8: Velocity Vectors about Corner.

The results shown in figures 5-7 and 5-8 were generated using the triangular grid partially illustrated in figure 5-3.

In the far left corner of both figures 5-7 and 5-8, there is a pressure build up that is consistent with the geometry. A hard change in direction the flow is essentially stagnant in the corner, and the increased pressure causes the fluid to turn in conjunction with the geometry, as expected. This feature is particularly important because it assists in turning away fluid from the gap between the ring and the barrel, the geometry on the far left in both figures 5-7 and 5-8. Therefore, the flow in the gap should be close to zero, which is the case as evident in figure 5-9, an illustration of the flow in the gap.

Figure 5-9: Velocity Vectors of the Flow in the Gap.

Clearly, the flow in the gap is negligible, justifying its omission in the proceeding cases.

Mesh Selection

A major restriction imposed by FLUENT is that all the elements throughout the flow field must be roughly the same size, due to the remeshing scheme. Thus, the selection process for the optimal mesh evolves determining the average element size and utilizing GAMBIT to employ that element automatically. The use of one element size will smudge the contours in areas of large fluctuations. By reducing the element size, one can reduce the averaging, but increases the computational expense and some other error sources. The optimal mesh is a balance of both the positive and negative aspect of a single element size.

The element selection process begins with a relatively large element, whose side is about (1mm), otherwise known as element size 1. That size is increased and decreased by a factor of 2 until an optimum value size becomes apparent. Figure 5-10 shows the various mesh sizes tested, starting with an element 2 times larger than element size 1 on the far left,

Figure 5-10: Various Element Sizes

ending with a case whose elements are one quarter the size of element 1 on the far right.

When the goal is to examine the behaviour of the valve, monitoring the force on the ring is a must, and figure 5-11 does just that. It plots the net force profiles of the drag acting on the ring as a function of time, generated by the various element sized meshes. The smoothest profile is that of element size 1. The case which utilized elements double that size

has small fluctuations throughout the entire spectrum, which is directly attributed to the coarseness of the mesh. Both cases with the smaller element sizes show a smooth profile until the later stages of the simulation, at which point significant fluctuations occur. As the simulation progresses, the ring begins to close the valve as per the design. The result is an

Figure 5-11: Variation of the Force on Ring due to Different Element Sizes.

acceleration of the flow in that region due to the decreasing area. Therefore, the flow conditions become more extreme with time, and hence the influence of various sources of error is greatly increased. One such source of error is that of truncation. The small time step sizes and the decreasing element sizes coupled with increasing flow complexity make truncation error significant in the later stages. Proof that it is in fact truncation error arises due to the fact that utilizing double precision greatly reduces the size of the fluctuations.

The fluctuation themselves are most likely caused by the skewed element arising from the mesh motion. The skewed elements are then remeshed, that is eliminated, in the following time step. However, over a single time step those elements can act as an impulse of error, which cause the fluctuations. Therefore, larger element sizes can deal with larger mesh motion without distorting the mesh, reducing the occurrence of skewed elements. It is important to note that the fluctuations are dampened quickly, which is directly linked to the high viscosity value. Decreasing the viscosity greatly increases the amplitude and transient life of the fluctuation.

The error is smoothed further by the small time step size as shown in figure 5-12. It

Figure 5-12: Variation of the Ring Velocity due to Different Element Sizes

illustrates the ring velocity as a function of time. In the net force on the ring plot, the variation between cases average about 10%. This is not an indication of error because it includes all of the fluctuation points in the average. As for the ring velocity plots, the variation averages about 1%, showing greater consistency in the results. Furthermore, corresponding results show that all of the meshes provide good results as per the motion of the ring; error is dampened and levels out.

Therefore, to choose an optimal element another factor comes into play, the computational expense. The two larger element sizes tested converge quickly in 2D and more importantly converge reasonably quickly when applied to a full 3D model. Conversely, the two smaller meshes are computationally expensive even in the 2D model. Larger elements have another price, when meshing complicated geometry, such as with the flute channels in the valve stud (found in the full 3D model), can result in skewed elements. In the end, element size 1 is found to be the optimal mesh. It provides good results, handles mesh motion with limited mesh deterioration and performs well in the 3D model.

Time Step Reduction

The closure of the valve occurs quickly, in the order of a few milliseconds, and so the time step must be very small. Common practice used to determine the optimal time step involves continual reduction of the time step size until the solution profiles from successive cases correspond. A good starting point for this particular valve is 5×10^{-5} sec, which places a reasonable amount of data points in the initial acceleration of the valve, expressed by the small lump to start the force profiles. Reduction of the time step takes place up to 5×10^{-7} sec, and the resulting force on ring profiles are shown in figure 5-13 and 5-14. The smaller the time step should help performance of the remeshing algorithm by

reducing the mesh motion, results consistent with the finding shown in figure 5-13. However, at a certain point in the time step reduction process, the results begin to fluctuate, and these cases are shown separately in figure 5-14.

Figure 5-13 Force on Ring Profiles with Varying Time Step Size.

Figure 5-14 Force on Ring Profile with Very Small Time Step Sizes.

Upon further inspection of figure 5-13, the first three cases show good correspondence. The largest time step (5×10^{-5} sec), as one might expect, has the most discrepancy, especially towards the end. In fact, this case ends significantly earlier in comparison to the other cases. As the ring begins to build up speed, the mesh motion per time step increases, so that it exceeds the capabilities of the remeshing algorithm. Therefore, the time step size (5×10^{-5} sec) is too large, suggesting the use of a smaller value. The following two cases of figure 5-13 correlate so well enough to suggest time step convergence, and so either time step would be a suitable choice for further cases.

One area to note in the case with time step 5×10^{-6} sec of figure 5-13 is that, toward the later stages of the simulation, small fluctuations begin to appear in the results. When considered with the results of figure 5-14, cases with even smaller time step sizes show that the fluctuations get worse with time, suggesting the source of error is truncation. Smaller time steps mean more truncation error and perhaps, more importantly, many more iterations for that error to propagate. Furthermore, the larger time step tends to more quickly dampen out error in the force profile. One possible reason for this phenomenon is the averaging nature of larger step sizes. Errant force values cause the model to compensate in the following time step, and hence the onset of the transient response. With smaller step sizes, the longer the periods between remeshing and thus increasing the period and influence of a skewed mesh. Figure 5-15 shows a closer view of the force on the ring using various time steps. It shows the smaller the time step the longer the fluctuation periods and the larger the amplitude of these fluctuations.

Figure 5-15: Close Inspection of the Force Profile with various Time Step Sizes.

On the positive side, the error is self correcting and even at its worse does not stray relatively far. Furthermore the strengths of the small time steps in other results such as the ring velocity shown in figure 5-16.

Figure 5-16: Ring Velocity with Various Time Step Sizes

The time step negates the effects of even the worst fluctuation, as seen by the smooth velocity profiles.

In the end, the time step size of 1×10^{-5} sec is the best choice for further cases. It generates the smoothest force profile, corresponds well with the other time step sizes, and is less computationally expensive than the next best option of 5×10^{-6} sec.

Effect of Ramp-up

Step function in CFD creates issues due to the sudden change. A step function itself is an ideal profile, and in the real case there must be some transition. The desire velocity profile of the valve assembly is a constant 2.5 m/s. To avoid a step function at the start-up of the simulation, a small acceleration period is present. Adding the acceleration period is known as ramping-up the velocity value, a common practice in CFD. Figure 5-17 illustrates three velocity profile possibilities for the start of a simulation. Running cases with these

Figure 5-17: Valve Assembly Velocity Profiles.

valve velocity profiles will show the problems associated with a unit step, and demonstrate the change with two ramp-up profiles, a linear version and a more gradual polynomial case.

In the eyes of a CFD program, a constant velocity profile will impose an impulse acceleration and force over the first time step. Previously mentioned, small deviations in the force value have sent the simulation into a transient response, and so large impulses in force must cause a violent transient response. The massive fluctuations are quite apparent in figures 5-18 and 5-19, which show the force and velocity profiles of the ring for the three cases respectively.

Figure 5-18 Force on Ring with Various Ramp-up Profiles

Figure 5-19: Ring Velocity with Various Ramp-up Profiles.

As anticipated the constant velocity profile does show a very strong transient response, with the amplitude of the first spike being over 100 kN. The linear case also exhibits minor fluctuations, but with much lower amplitude due to the greatly reduced initial applied velocity after the first time step. The polynomial profile further reduces the initial velocity and thus shows no such fluctuations. The large spikes or fluctuations at the start of the simulation are a numerical response which is strong enough to display effects in the velocity results, whereas previously the small time step was able to smooth out the fluctuations.

The system does manage to dampen out the transient response and shows no ill effects in the profile shape later in the simulation. However, the problem that does arise with the large fluctuations is that they induce large changes in position of the ring. This extreme mesh motion will in many cases surpass the capability of the remeshing and thus

prematurely kill the simulation. Therefore, to eliminate the spike the polynomial profile is the ideal candidate.

Towards the end of the simulations, it is apparent in figures 5-18 and 5-19 that the profiles do not match, the rapid velocity increase occurs earlier in the constant velocity case. The predicament arises because the valve in the constant velocity case experiences twice the acceleration compared to the other two cases. A fact which is evident in figure 5-17, where the area of the two ramp-up cases is half of the constant velocity case. Knowing this fact, one can retard the timing of the first case by half the acceleration period so that the ring's position for all three cases will be identical. Doing so should generate identical profiles, as shown to be true in figure 5-20 and 5-21. Therefore, the only effect of adding a ramp-up on the results is that one half the acceleration period is added to the overall time of the valve closure.

Figure 5-20: Force on Ring with Various Ramp-up Profiles with time correction.

Figure 5-21: Ring Velocity with Various Ramp-up Profiles with time correction.

2D Axisymmetric compared to full 3D model

As stated earlier, the main difference between models is the inclusion of the flutes in the valve head in the 3D model. Adding the third dimension exponentially increases the computation time. It also has an effect on the ring profiles as well, as shown in figures 5-22 and 5-23.

Figure 5-22: Force on Ring Profile for 2D axisymmetric and full 3D model.

Figure 5-23: Ring Velocity Profile for 2D axisymmetric and full 3D model.

Again, the shape of the profile is very similar but the discrepancy suggests the 2D axisymmetric model underestimates the force acting on the ring. The flutes on the stud channel accelerate the flow in front of the ring due to the constricting area. No such acceleration occurs in the 2D axisymmetric model. This faster moving flow will generate a slightly larger force on the ring. Furthermore, a small portion of the flow will pass over and around the valve head, picking up speed in the process. This flow then runs into the ring causing a change in direction. The momentum transfer of the change in direction results in an extra force helping to close the valve, which is also not accounted for by the 2D axisymmetric model. Both scenarios described are visible in figure 5-24, which shows plane cutouts of the velocity counters in the full 3d model. It shows the flow through the flutes in one plane and around the head in another.

Figure 5-24: Velocity Contours in 3D model.

It becomes obvious why the valve closure occurs faster when modelled in 3D, the fluid velocities are higher on the valve stud. Figure 5-25 shows the equivalent contours using the 2D axisymmetric model. The downstream contours

Figure 5-25: Velocity Contours using 2D axisymmetric model.

towards the rear of the ring remain similar in between models.

Prior to the comparison of 2D to 3D profile, discrepancies were expected. The role of the 2D axisymmetric model is help save time in determining the optimal mesh size and time step. The optimization process is not affected based on an underestimation of the force on the ring. As per the validity of the results neither, the 2D nor 3D can be shown to be more valid without the support of experimental data. However, the 3D model should provide better results when the magnitude of the results is important because it does incorporate more of the geometry features of the valve. Moreover, the focus in this study is to determine the effect of altering certain parameters whilst attempting to gain a knowledgebase of the valve motion, almost all of which can be done utilizing and underestimation force values. The idea that altering certain parameters has the same effect on both the 2D and the 3D model generated profiles will be further supported by upcoming results. Attempting to justify the use of the 2D axisymmetric model is not to justify not using the 3D model, but instead to show that it is a valid tool to be used in conjunction with the 3D model to help save time.

Valve Operation Results

Where the previous section is geared towards validation, here the simulations represent actual valve closure. The case variations occur by altering one or two input parameters in order to determine its role and influence on the closure of the valve, namely the movement of the ring.

Baseline Results

As a platform for comparison, a baseline case is necessary. This case should be simple, in that it utilizes the minimum input and yet provides a realistic representation of the actual valve motion. For instance, as shown in table 3.1, there are many inputs in the area of material properties but the density, 1.83 g/cm^3 and the viscosity, $0.0012 \text{ m}^2/\text{s}$, are necessary for the baseline run. The internal pressure is set to 30 MPa and the valve assembly is set to travel at 2.5 m/s constant speed, with a small ramp-up acceleration portion. The downstream nozzle is replaced by a pressure outlet boundary condition, with a 50 Pa back pressure value. The nozzle replacement is explored further in an upcoming section examining back pressure influence.

Given the input just mentioned, the resulting force acting on the ring during the simulation is shown in figure 5-26. The first noticeable feature is the effect of ramp-up,

Figure 5-26: Baseline Force Profile.

where the acceleration of the ring mirrors the acceleration of the valve assembly, but in the opposite direction. As the valve moves forward, the surrounding fluid is forced to move as well. Fluid traveling forward towards the nozzle encounters the resistance in the form of pressure due to the nozzle area restriction. Hence, the fluid will be more inclined to travel in the opposite direction, over the ring, and as it does, the fluid is forced to change direction due to the geometry. That change in direction causes pressure variations which drive the free moving ring to close. Figure 5-27 shows the pressure contour over the entire domain and it illustrates a high pressure in front of the valve and low pressure behind the valve.

Figure 5-27: Pressure Contours Over Entire Domain.

The next major feature of figure 5-26 is that the force acting on the ring is exponentially increasing as a closure force. Examining the velocity of the fluid in the domain sheds light as to why, and it is shown in figure 5-28. This figure shows the valve stud

Figure 5-28: Velocity Contours Over Entire Domain.

imparting its velocity on the fluid directly in front of the valve, where it then tends to curl over the edge and make its way past the ring. As the flow nears the rear of the valve the passage area is being constricted by the ring as it closes, a feature which accelerates the flow in this region. The flow acceleration is compounding because the ring continues to close, thus ever increasing the velocity of the flow here. Soon after passing the ring the flow is forced to turn sharp, creating a curl in the flow. A curl is always accompanied by a low pressure spot. As the flow accelerates by the ring the curl gets stronger and the pressure behind the ring decrease. The pressure variation is driving force of the ring and is exponentially increasing, consistent with ring drag plot. The velocity vectors plots highlighting the curl behind the ring is given by figure 5-29, and is accompanied by a contour pressure plot of the same area in figure 5-30.

Figure 5-29: Velocity Vectors at Rear of Ring

Figure 5-30: Pressure Contours Near Rear of Ring.

A direct result of the force acting on the ring is the resulting ring velocity, shown in figure 5-31. This again shows the effect of ramp-up and the exponential increasing closing force experience by the ring as the simulation progresses.

Figure 5-31: Baseline Ring Velocity Profile.

Plastic Material Properties

To gain some insight into the role of the certain material properties, a case is run with altered properties values. The two main differences involve the value of density and viscosity. To make comparisons, a good choice for new material properties should be that of a commonly used material in injection molding, that is thermoplastics. Common thermoplastics include ABS, Nylon, Polycarbonate, Polypropylene, Polystyrene and so on. The range of densities for these plastics is given in Table 4-1.

PLASTICS	DENSITY (G/CM ³)
ABS	1 – 1.05
PA	1.13 – 1.35
PC	1.2
PP	0.905
GPPS	1.05

Table 5-1: Common Injection Molding Thermoplastics Density.

Instead of deciding on a specific plastics and its value for density, an average value of (1.00 g/cm³) is chosen. The idea is that that density value is of a common thermoplastic, representative to the various plastics listed. The viscosity is set to (1e-6 m²/s); a value is consistent with the fact that the plastic is at high temperature and that the injection process for thermoplastics is a turbulent flow.

During the valve closure process the only link between the ring and the rest of the valve assembly is the fluid itself. The density of the fluid is a measure the stiffness of the link between the two components, and thus the higher the density the larger the transfer of momentum from that valve assembly to the ring. In other words, the forces acting on the ring should be higher when utilizing the magnesium alloy as the injection material because it is denser than the plastics. A results comparison of the baseline data with that of cases utilizing the plastics material properties, as shown in figures 5-32 and 5-33, is consistent with the expected role of the density parameter. The higher transmission of force is clearly visible, especially in the ramp-up of figure 5-32. As a results valve closure speeds are quicker with increasing density. When considering valve life, these results are especially important. Injection molding is a cyclic process, and so by significantly increasing the force on the ring during a single cycle will also decrease the life of the valve significantly.

Drag on Ring for Different Materials

Figure 5-32: Force on Ring with Different Material Properties

Ring Velocity with Different Materials

Figure 5-33: Ring Velocity with Different Material Properties

The data in figures 5-32 and 5-33 show both results generated using the 2D axisymmetric model and the full 3D model. As mentioned earlier the effect of changing certain parameters should be consistent between models, and it is. The gap between the baseline and plastic cases is the same in size in the 2D axisymmetric model and the 3D model. Furthermore the underestimation of force is consistent in both the baseline and the plastic property results. Again illustrating the value of the 2D axisymmetric model.

Effect of Thermal Properties

The main goal here is to explore the effect of using the thixotropic material. FLUENT itself cannot model millions of individual solidus particles suspended throughout the fluid. It can however monitor the solidus mass fraction and provide a corresponding contour plot, based on the temperature contours and the thixotropic material properties listed earlier in table 3.1. The mass fraction contour plots can provide insight as to which areas are susceptible to solidus particle build up.

A comprehensive thermal model of the thixomolding valve requires more research into various aspects of the thixomolding machine. For example, the size of the mold will affect the shot size, and thereby alter the amount of time fluid is subjected to the heater bands. Other factors include the heater band width, the applied temperature distribution on the barrel, the screw rotation speed, all of which have an effect on the temperature profile. Exploring these factors is beyond the scope of this thesis, instead only one set of thermal input parameters is chosen. The heater bands are fixed at a width of 2 cm with a 0.5 cm gap between them. These bands are set at 853 K, the desired melt temperature. The incoming melt, that is fluid at the end of the screw compression, is set at few degrees cooler, 850 K. The cooler incoming melt is consistent with the thixomolding process outlined earlier

because some heating of the melt occurs during screw recovery, at which point the fluid is filling the area in front of the valve. Figure 5-34 depicts the steady state temperature contours of the valve model given the input conditions just mentioned.

Figure 5-34: Temperature Contour at Start of Valve Closure.

The temperature contours given are what one would expect. The cooler incoming melt is given in blue and is quickly heated because the fluid is in close proximity to the heater bands and it moving at its fastest here. By the time it passes by the along side of the ring, the flow is at about 852 K, already close to the desired melt temperature. The heater bands themselves are depicted as the hot spots on the barrel, and their position is visible due to the slight lull in temperature consistent with the gap between heater bands.

The only area of concern is the rear seat, where the ring impacts the valve assembly. Here the liquid fraction is about 2% lower, not a large value but that number is directly

related to the incoming melt temperature. Lower the temperature and liquid fraction value may become significant. A closer depiction of the rear seat and the liquid fraction contour is given in figure 5-35.

Figure 5-35: Liquid Fraction near the Rear Seat.

The temperature profile of figure 5-35 becomes the starting point of the rest of the simulation involving the closure of the valve. The closure process is same as previous case except for the inclusion of the energy equation to encompass the added thermal input. As per the effects of the added thermal complexity on the ring drag and velocity profiles, the results are given in figure 5-36 and 5-37 respectively. Clearly there is no significant change; the increased geometry and thermal complexity shown a slight increase in numerical error fluctuations, which one would expect. The fluctuations do smooth out in the velocity profile, and thus are relatively insignificant. A positive arising due to the fact that the profiles remain unchanged is that the other cases which omit the thermal properties are still realistic.

Force Acting on Ring

Figure 5-36: Force on Ring including Thermal Effects.

Ring Velocity

Figure 5-37: Ring Velocity including Thermal Effects

The affect of the valve motion on the temperature contours is given in figure 5-38. During valve closure the downstream, hotter melt leaks towards the back of the ring and the upstream colder melt is heated in the process. This would dispute the idea of solidus particle build up on the rear seat. The heating effect and the direction of leakage flow would tend to remove solid particles build up on the rear seat.

Figure 5-38: Change to Temperature Contours due to Valve Motion.

Barrel Pressure

To reduce the computational size of the model the nozzle is omitted. Depending on the shot size the nozzle can be a significant distance from the valve. Rather than having a long barrel in the model the nozzle is replaced with a pressure outlet. The effect of a nozzle is to accelerate the flow increasing the upstream pressure in the process. Figure 5-39 shows the pressure contours of a simulation involving just the nozzle. To the left is a velocity inlet and

Figure 5-39: Nozzle Effect on Pressure Field.

on the left is an outflow boundary condition. Clearly, the upstream pressure is constant and increased by about 322Pa, given that the input velocity is 1m/s. The inlet of the nozzle case is the outlet of the valve model, and so it is justified using a pressure outlet enforcing a small back pressure.

The next logical progression is to determine the role of the back pressure. Therefore, a few cases with increasing back pressures are compared to a case with no back pressure and one with a vacuum pressure. Eliminating the effect of the nozzle, that is the

back pressure, can be done by using a slightly lower internal pressure in the mold. The vacuum pressure negates the pressure build up of the nozzle.

The force acting on the ring as generated with the various back pressure conditions is given in figure 5-40. Up to this point, the effects on the drag profile have maintained the same shape, at best altering the timing of closure. Here, back pressure is shown to be very

Figure 5-40: Force on Ring with various Back Pressures.

influential to the ring motion. For the first time the ring in some cases travels alongside the valve in the positive direction. With no back pressure, the fluid flow direction is that of the main valve assembly, thus imparting a positive force on the ring. Adding vacuum pressure accelerates the flow in the positive direction, amplifying the positive force on the ring. For the case with no back pressure, once the ramp-up portion of the simulation ends, the speed of the main valve assembly begins to funnel fluid past the rear of the ring, thereby inducing the exponentially increasing closing force. Thus, the ring begins to decelerate, a trend which is more visible in the ring velocity profile plot shown in figure 5-41. As for the vacuum case,

Figure 5-41: Ring Velocity with Various Back Pressures.

there is a balance between the vacuum pressure and the force generated by fluid leaking past the ring, thus the constant velocity shown by the ring velocity profile of that case. In regards to cases with a back pressure, the ring profiles follow those of the baseline results. The magnitude of the back pressure does not alter the profiles.

The optimal profile is that of the case with no back pressure. The initial forward velocity greatly reduces the ring velocity at impact, while only slightly increasing the time required for valve closure. Reducing the impact velocity can extend the life of the valve and also reduce the chances of ring bouncing effect, a plausible development should the impact velocity be high enough. A bounce would cause a significant amount of flow to leak past the ring because of the high pressures and the high acceleration of the flow through small gaps.

Other profiles which provide further insight towards the role of back pressure and at the same time evidence to support the drag and velocity profiles of the ring are given by

the leakage velocity and the melt injected velocity. Figures 5-42 and 5-43 are the leakage flow and injection flow profiles, respectively. Be it that the flow is incompressible and that

Figure 5-42: Velocity of Leakage flow (Back Pressure cases).

Figure 5-43: Barrel Injection Velocity (Back Pressure cases).

the areas are unchanging, the two figures are in essence a representation of the mass flow leaking past the valve and that which is injected into the mold. In the case where back pressure is present, the majority of the flow leaks past the ring generating the large closing force. The case with equal pressure has a moderate amount of flow in both directions. Some leakage is good, it quickens the closing time of the valve and also helps eliminate solidus particle build up on the rear seat.

Input Velocity Profile Alterations

The input velocity is the motion applied to the valve assembly. It can be given various profile shapes; in other words, it is not restricted to a constant velocity, such as 2.5 m/s, in the baseline case. Altering the profile shape will help determine the effect that acceleration has on the main valve assembly has on the free moving ring. Figure 5-44 illustrates the profiles to be used in the simulation here. The new or altered profiles have a period of acceleration followed by a deceleration period. The total acceleration experienced

Figure 5-44: Various Stud Velocity Profiles.

by the assembly is constant and is how the peak velocities are determined. The new profiles are categorized by the amount of time spent accelerating. Previously, the ramp-up portion of the baseline results was shown to offset the results by one half the ramp-up time. Due to the fact that the acceleration is totaled without compensating for the ram-up results, the altered profile results are themselves offset to compensate.

As per the results of the simulations, the drag profiles on the ring are given in figure 5-45. Here, the offset of the results is clearly visible, in that they start half way through the ramp-up portion of the baseline results. The figure also shows a unit step function for the force initially, consistent with the constant acceleration imposed on the valve assembly.

Figure 5-45: Force on Ring with various Input Profiles.

Towards the end of the acceleration period, the unit step shape begins to curve slightly. In essence, this illustrates that the force acting on the ring is a combination of the acceleration

force imposed on the valve and the force generated by the fluid motion passing the ring. Interestingly, once the deceleration period begins, the all ring drag profiles revert back to that of the baseline results, a fact easily explained because each of the imposed accelerations has a corresponding deceleration which causes the total acceleration to be consistent between cases. Therefore, the fact that the total acceleration is constant causes the negative unit step generated by a deceleration portion to negate the positive unit step created by the acceleration, and hence the force profiles revert back to the baseline profile which has no acceleration on the valve at this point.

Ring velocity also mirrors a combination of the effect of the valve acceleration and the acceleration generated by the fluid motion, as shown in figure 5-46. The first portion is governed by the valve acceleration and that is followed by the deceleration portion bringing the profiles back to that of the baseline results. All the while the effect of the fluid motion is exponentially increasing the speed at which the valve closes.

Figure 5-46: Ring Velocity with various Input Profiles.

Despite the different profiles, the time of valve closure remains the same, governed mainly by the total acceleration and not the method or profile at which it is applied. In the end, the velocity profile of the valve assembly is of little significance to the valve life because the pressure forces generated near the end of valve closure are much greater than those caused by the acceleration of the main valve assembly.

Design Alterations

The next logical step to parameter alterations is changing that actual geometry. There are many possible changes options available, so to narrow the selection band only the ring entry and exit angle will be altered. In other words, the valve geometry alterations are limited to changing the shape of the leading edge and the trailing edge of the ring.

Ring Rear Angle Geometry Alterations

The original trailing edge angle of the valve is set to 75° to the horizontal. The extreme cases involving altering this angle involve setting the angle to 90° , completely upright, and 45° , while two intermediate values are 70° and 80° . Changing the rear ring angle also requires altering the rear seat angle to match so that the two surfaces are aligned to allow valve closure. The resulting drag and velocity profile of the various ring shapes are given in figure 5-47 and 5-48, respectively. The resulting profiles show that the steeper the rear ring angle the faster the valve closes. The sharper ring angles impose a sharper change in direction for the fluid, which causes lower pressure behind the ring due to the stronger curl in velocity. Initially, the flow is slow moving fluid and imposes the same force on the ring. Later in the simulation, as the flow gains speed, the effect of the rear ring angle should be and is more influential.

Figure 5-47: Force on Ring Profiles with Rear Angle Alterations.

Figure 5-48: Ring Velocity Profiles with Rear Angle Alterations.

Ring Front Angle Geometry Alterations

The front ring angles are measured to the vertical. For example, figure 5-49 shows a 10° alteration to the front of the ring. Other cases include one with 25° and a negative 10°

Figure 5-49: Ring Geometry with a Front 10° Change.

ring front angle. The negative angle is not a good design because it would funnel flow towards the gap between the ring and the barrel, but is included for thoroughness.

The resulting drag and velocity profiles of the various ring shapes are given in figures 5-50 and 5-51, respectively. Clearly visible is that there is no real change in the profiles given the altered front ring angle, a result which is odd because the rear angle had significant influence. The exclusion of valve tip inherent in the 2D axisymmetric model may be the cause.

Figure 5-50: Force on Ring Profiles with Front Angle Alterations.

Figure 5-51: Ring Velocity Profiles with Front Angle Alterations.

Therefore the 10° case is repeated using the full 3D model, and the resulting drag and velocity profiles are given in figures 5-52 and 5-53.

Figure 5-52: Drag Results of Ring with Front 10° Alteration and modeled in 3D.

Figure 5-53: Velocity Profile of Ring with Front 10° Alteration and modeled in 3D.

Obviously, the effects of the valve tip are significant because the valve is shown to close quicker. The increase in the force on the ring is due to the easier flow passage past the ring. The slight change in angle acts as a funnel for the flow near the barrel, otherwise not directed past the ring with the flat design of the original geometry. Once again, the extra flow lowers the pressure behind the ring and thus increases the pressure force imposed on the ring. A larger angle for the front of the ring will definitely amplify the influence of the geometry and hence further quicken the valve closure time.

Chapter 6 Conclusion

In an attempt to analyze the dynamics of a non-return ring check-valve during operation, more specifically valve closure, many simulations were run. A model was developed which allows for manipulation of a variety of variables with the intent of isolating the role and influence of a particular variable. With such a tool it is possible to determine which variables are suited to optimization and also highlight problematic areas or design shortcomings.

A good portion of the simulation results were geared toward the validation of the model, a necessary step due to the lack of experimental data. Common to CFD problems, the two methods of validation include a mesh analysis and time step convergence tests. In both tests the results showed good convergences, suggesting that, for the given physical setup used, the model provided accurate results. There were a few fluctuations in the ring drag profiles but they were shown to dampen quickly and have no altering effect on the profiles themselves. Furthermore, the final selection of time step size and element size used for any subsequent cases took into consideration both minimizing the fluctuations, as well as the computational expense, thereby minimizing error.

In regards to validation of the physical model, several simulations were run with this goal in mind, one of which involved gathering evidence to support the omission of the gap between the ring and the barrel. It was shown that the mass flow through this gap was very minimal and also that neglected viscous forces were insignificant because the pressure forces acting on the ring were so high. Another area to address is the small acceleration period of the valve body, previously labeled ramp-up. Adding it to the velocity profile of the valve

body was shown to greatly improve the convergence during simulation of the early results. In fact, ramp-up was essential in making some simulation solutions possible. Moreover, the ramp-up feature was shown to have no effect on the profile shape of the results being sought after, namely, the resulting motion of the ring.

One area of the physical model which could be improved is the viscosity representation, which was set to a constant value, when in actuality it is temperature dependent. However, the value used is not a bad representation. There is evidence that shows thixomolding is a laminar process, whereas most plastic injection molding is a turbulent process. When a case was run with the properties of a plastic, that is, lower density and viscosity values, some significant fluctuations arose towards the end, when the fluid became accelerated. Therefore, the error in the results for the plastic case became more evident as the velocity of the fluid increased, as well as the fact that there was more difficulty in converging of the results. The sudden rise of fluctuations at a certain flow speed suggests that the fluid might have become turbulent and so the laminar physical model used is no longer accurate. Now, because no such phenomenon occurred with the magnesium alloy properties, it would suggest that these cases remained laminar, thus providing evidence that the viscosity value had some accuracy, laminar flow being a very important part of the physical model.

Examination of the motion of the ring during valve closure without any thermal effects was labeled the baseline results and was the standard that all other variable manipulations were compared to. Basically, the valve body was set into motion at a constant speed, meanwhile the pressure and velocity flow fields, as well as the dynamics of the ring, were monitored. The results themselves were shown to be logical, given the geometry, and easily explained using simple CFD cases such as a backward facing step and duct flow around corners. It was found that pressure contours generated by the valve body motion, coupled

with the backpressure generated by the nozzle, drive the motion of the ring in such a manner that the closing force is exponentially increasing. The acceleration forces of the valve body are transferred to the ring but are overrun by the pressure force in the later stages of the simulation. The problem with these results is that they suggest a high speed impact of the ring into the rear seat of the valve body. High speed impact would indicate a transient response after collision, that is bouncing of the ring off the rear seat. The bouncing behaviour would allow further leakage of the melt, a situation which should be minimized. Additional research into the bouncing behaviour would be another possible initiative.

The plastic material properties simulation alluded to earlier gave some valuable insight into two key parameters, density and viscosity. It was shown that the density is a measure of the stiffness of the link between the ring and the rest of the valve body. The denser the fluid, the more momentum is transferred from the valve body to the ring. The high density of the magnesium alloy imparted greater forces to the ring throughout the entire valve closure process. Therefore, increased forces on a cyclic process means a reduction in the life of the valve as a function of increased density. As for the viscosity, it was shown to providing damping, touched upon earlier.

In an attempt to include more complex aspects of the thixomolding process, some thermal properties were added to a set of cases. The added heater bands and varying temperature contours showed no significant effect on the valve motion. However, the results did suggest that some leakage may be a positive. Due to the fact that the downstream melt is hotter, leakage of this material will heat cooler incoming melt; a fact disputing the notion of solidus build up behind the valve as a means of inhibiting proper seal between the ring against the rear seat. This is not to say that the build up of solidus material behind at the critical juncture is not possible. It is possible that the temperature difference between

upstream and downstream melt may be greater than the one imposed in the simulations. The temperature difference and the low speeds about the corner of the rear seat are the necessary ingredients. Furthermore, the phenomenon may be a longer term effect, occurring after many iteration of the thixomolding process and not visible in a single case. Therefore, another aspect of the valve model subject to future work would be an exploration of the long term affects. One would make the model to simulate the entire cycle and then analyze the results after hundreds of iterations. A final note on the thermal aspects utilized in the simulations, their influence might be more significant if the viscosity were made temperature dependant.

Another area of the valve model explored was the effect of the nozzle. It was shown to induce a slight build up of pressure upstream, in other words, it created a back pressure. The valve model utilized a pressure outlet with a back pressure condition to simulate the nozzle, thereby simplifying it whilst remaining consistent with affects of the nozzle. That leads to exploration of the role of pressure at the outlet with three scenarios, one with back pressure, one with no pressure difference and the final with a vacuum scenario. It was found that the pressure at the outlet governed the direction of flow past the ring. In a back pressure condition, the flow traveled in the negative direction, that is, it leaked past the ring, thereby closing the ring faster. The vacuum case was the opposite, whereby the flow moved in a positive direction. With no pressure difference, the valve still closed but not with a much lesser velocity at impact, an ideal scenario. The problem arises in that it would be very difficult to eliminate the pressure difference. It would entail balancing the vacuum pressure of the mold to equal that which is generated by the nozzle. The back pressure at the nozzle is based on the incoming flow conditions which have many determining factors, thus making it difficult to predict. Furthermore, the results showed that the strength of the

back pressure is irrelevant such that a small variation is enough to induce the exponentially increasing closing force. These factors make the elimination of back pressure difficult; however, if accomplished it would eliminate the bouncing of the ring. One might think that creating a control loop that measures the mold pressure and the barrel pressure and then adjusts the mold pressure to match would be a solution; however, making the mold pressure value dynamic, especially over such a small period of time, is impractical. The vacuum scenario is also not a good choice because colder melt is drawn forward, changing the consistency of the melt, as well as enhancing the possibility of rear seat solidus particle build up. In the injection process the melt must be pushed into the mold and not sucked, thereby maintaining control.

In regards to the role of the valve body motion affect on the ring, it was found that the total acceleration, and not the path, determined the valve closure time. Altering the velocity profile of the valve body in a set of cases illustrated that the ring motion mirrors that of the valve body until a certain point at which the pressure force begins to dominate. The result is a motion of the ring which is similar to that valve body for the first portion of the simulation, followed by a sharp increase in the closing speed of the ring, leading to impact.

The final aspect explored is that of the ring shape. Both the rear and front edge angles were altered. For the rear angle, the sharper the turning angle of the flow, the quicker the valve closed, the cause being that, as the turning angle increases, so too does the pressure drop behind the valve; the lower the pressure behind the valve, the higher the closing force, and thus the quicker valve closure time, consistent with the results. Making the angle steeper minimizes the leakage in one respect because the valve closes quicker and the flow is more restricted moving towards a sharp change in direction. However, it does increase the change of ring bouncing. Other factors important to rear angle optimization include the ease of

flow past the ring during recovery (melt accumulation) and stress tolerances due to higher impacts speeds.

Modeling change to the front angle of the ring required the use of the full 3D simulation in order to include the effects of the valve stud. When this angle is perpendicular to the barrel, it was shown to impede flow in the leakages direction. Therefore, slightly altering the front angle increases the closing speed of the valve by funneling more melt past the ring, inducing the exponential closing force faster.

When all is said and done, the plethora of results provides a great deal of insight into the inner workings of the one-way ring check valve. Moreover, they provide many avenues of possible design optimization, as well as a few topics of possible future research. One of the best avenues for improvement to the model would be experimental data for validation purposes and also augmentation of the CFD physical model. As it stands, one is left with a good valve modeling tool which provides comprehensive results and is versatile in that it can be easily adapted to other valve designs, such as the ball check valve.

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Appendix

UDFs

Valve body Motion

```
/******
 *
 * 1-degree of freedom equation of motion (x-direction)
 * compiled UDF
 *
 *****/
#include <math.h>
#include <stdio.h>
#include "udf.h"

DEFINE_CG_MOTION(head, dt, vel, omega, time, dtime)
{
    real vhead;

    if (time<0.00025)
        {vhead = -time*(416.66667-time*(125000000-
333333333333.39800*time));}
    else
        {vhead = 2.5;}
    Message ("UDF head: vhead = %f\n", vhead);

    vel[0] = vhead;
}
```

Ring motion

```
#include <stdio.h>
#include "udf.h"

#if !RP_NODE
# define UDF_FILENAME "udf_loc_velo"

/* read current location and velocity from file */
static void
read_loc_velo_file (real *loc, real *velo)
{
    FILE *fp = fopen(UDF_FILENAME, "r");

    if (fp != NULL)
    {
        float read_loc, read_velo;
```

```

        fscanf (fp, "%e %e", &read_loc, &read_velo);
        fclose (fp);

        *loc = (real) read_loc;
        *velo = (real) read_velo;
    }
    else
    {
        *loc = 0.0;
        *velo = 0.0;
    }
}

/* write current location and velocity in file */
static void
write_loc_velo_file (real loc, real velo)
{
    FILE *fp = fopen(UDF_FILENAME, "w");

    if (fp != NULL)
    {
        fprintf (fp, "%e %e", loc, velo);
        fclose (fp);
    }
    else
        Message ("\nWarning: cannot write %s file", UDF_FILENAME);
}
#endif /* !RP_NODE */

DEFINE_ON_DEMAND(reset_velocity)
{
    #if !RP_NODE
        real loc, velo;

        read_loc_velo_file (&loc, &velo);
        write_loc_velo_file (loc, 0.0);

        Message ("\nUDF reset_velocity called:");
    #endif
}

DEFINE_CG_MOTION(valve, dt, cg_vel, cg_omega, time, dtime)
{
    #if !RP_NODE
        Thread *t = DT_THREAD (dt);
        face_t f;
        real force, loc;
    #endif
    real velo;

    /* reset velocities */
    NV_S (cg_vel, =, 0.0);
    NV_S (cg_omega, =, 0.0);

    if (!Data_Valid_P ())
        return;
}

```



```

#if !RP_NODE
  /* compute force on ring wall */
  force = 0.0;
  begin_f_loop (f, t)
  {
    real *AA;

    AA = F_AREA_CACHE (f, t);
    force += F_P (f, t) * AA[0];
  }
  end_f_loop (f, t)

# if RP_2D
  if (rp_axi)
    force *= 2.0 * M_PI;
# endif

  read_loc_velo_file (&loc, &velo);

  /* compute change in velocity */
  {
    real dv = dtime * force / 1;

    velo += dv;
    loc += velo * dtime;
  }

  Message ("\nUDF valve: time = %f, x_vel = %f, force = %f, loc(m)=
%f\n",
          time, velo, force, loc);
  write_loc_velo_file (loc, velo);
#endif /* !RP_NODE */

#if PARALLEL
  host_to_node_real_1 (velo);
#endif

  cg_vel[0] = velo;
}

```

8) 6-3-23