RESIDUAL STRESSES AND BIREFRINGENCE IN GAS-ASSISTED INJECTION MOLDING OF AMORPHOUS POLYMERS: SIMULATION AND EXPERIMENT

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This study presents measurements and simulations of the distribution of the birefringence components, $\Delta n$ and $n_{rr} - n_{\theta\theta}$, and the average birefringence, $\langle n_{zz} - n_{\theta\theta} \rangle$, and polymer/gas interface in polystyrene (PS) and polycarbonate (PC) spiral-shaped tubular moldings obtained by Gas-Assisted Injection Molding (GAIM) under various processing conditions. Furthermore, free quenching experiments in cylindrical samples were carried out at different initial temperatures, and various components of birefringence and stresses were measured and simulated. The flow- and thermally-induced stresses were simulated using linear and nonlinear viscoelastic theories, respectively. The flow- and thermally-induced birefringence components were calculated using the stress-optical rule and photoviscoelastic model, respectively. The governing equations of the GAIM process were derived using a nonlinear viscoelastic model and solved using a hybrid finite element/finite difference/control volume method. The governing equations to calculate the thermally-induced stresses were discretized using finite differences. The numerical results predicted qualitatively the effect of the processing variables on the polymer/gas interface distribution of the GAIM moldings. It was found that the processing variables that strongly affected the interface distribution were the injection speed, gas-delay time, and the shot size. The processing variables that exerted less influence on the polymer/gas distribution were the gas pressure and the melt and mold temperatures.
The processing variables that strongly affected the birefringence $\Delta n$ were the melt temperature, injection speed, and gas-delay time. The mold temperature, gas pressure and shot size exerted less influence on $\Delta n$. For PS GAIM moldings the measured birefringence near to the outer wall did not relax when a section was annealed at a temperature close to the glass transition temperature while the birefringence near to the inner wall did relax significantly. This observation was consistent with the idea that the birefringence at the outer wall was mainly induced by shear and normal stresses, while that at the inner wall was induced by thermal stresses. For PC GAIM moldings the measured $\Delta n$ and $n_{rr} - n_{\theta\theta}$ relaxed significantly near the inner and outer walls, suggesting that the thermally-induced stresses exerted a strong influence on the birefringence throughout the wall thickness. The simulated birefringence qualitatively described the measurements. Summation of simulated thermally- and flow-induced birefringence provided a better description of measured birefringence in PS GAIM moldings. However, for PC GAIM moldings, simulations showed large discrepancies. This was attributed to the strong influence of thermally-induced birefringence throughout the wall thickness of the molding.

Melt temperature, gas-delay time, and injection speed strongly affected the average birefringence in PS GAIM moldings while the shot size and gas pressure exerted less influence. For PS GAIM moldings the contribution of the thermally-induced average birefringence was minimal while for PC GAIM moldings it was significant.
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CHAPTER I
INTRODUCTION

In most polymer-processing operations, the polymer melt undergoes rapid deformations, high stresses, and fast cooling in order to keep a determined geometry. During the deformation of the polymer melt, owing to its viscoelastic nature, the total strain contains reversible and irreversible components which lead to the build-up and relaxation of stresses. The stresses generated while the polymer is flowing tend to align the molecules to the flow direction and, due to the rapid cooling process, stresses do not have time to relax after the flow cessation. This leads to a frozen-in molecular orientation and flow-induced residual stresses in the polymeric product [1, 2]. Polymer molecules have an intrinsic birefringence due to the difference between the polarizability in parallel and perpendicular directions to the molecular backbone [3]. This causes difference between the refractive indices along and across the molecule and, as a consequence, light travels with different speeds in those directions. When the molecules are randomly oriented in the polymeric part, it behaves as an isotropic medium. Therefore, the interaction of light with the molecules, on average, will be the same for any direction in the sample and any plane of polarization [4]. However, when the molecules are oriented in a preferred direction, the sample becomes anisotropic, exhibiting different refractive indices perpendicular and parallel to the optical axis, which transforms the plane
polarized light into elliptically polarized radiations. This phenomenon is called birefringence or double refraction of light [4]. Another important phenomenon that occurs during the solidification process is the inhomogeneous cooling that the polymer experiences throughout the part’s thickness which causes density variations and volume shrinkage. The combination of an inhomogeneous cooling and a strong temperature dependence of the mechanical properties of polymers are the main factors that generate thermally-induced stresses through the thickness of the polymeric part. The combined effect of flow- and thermally-induced stresses render a complex state of residual stresses in the final product. These residual stresses are the main source of birefringence in polymeric parts. Flow- and thermally-induced residual stresses result in flow- and thermally-induced birefringence, respectively [2]. The development of residual stresses and frozen-in molecular orientation are strongly influenced by the polymer rheology, polymer chemistry, and processing conditions.

Conventional injection molding (CIM) has been characterized as being a highly automated process which produces polymeric parts with accurate dimensions at rapid rates. It has been sufficient to produce most parts in different technological fields with necessary standards. However, for certain applications such as the production of hollow parts or those with hollow sections, CIM is not applicable. Therefore, improvements and modifications to this process have been developed to extend its ability for these applications. One of these technologies is Gas-Assisted Injection Molding (GAIM) which is, in essence, a process to produce polymeric parts with hollow sections. In CIM and related technologies such as GAIM, birefringence and residual stresses cause several post-molding problems such as warpage, shrinkage, crazing, thermally-induced
distortion, amongst others [1, 5]. Especially in GAIM, due to the complex polymer-gas interaction and the considerable number of processing variables such as: gas pressure, gas injection time, melt and mold temperatures, injection speed, geometric constraints, and the diversity of materials employed, the prediction of residual stresses and birefringence is quite complex.

The present study describes the attempt towards the modeling of gas penetration, residual stresses, and birefringence in gas-assisted injection molded articles and free-quenched samples of polystyrene and polycarbonate. Numerical simulation of the GAIM process, which includes polymer melt filling, gas penetration, and cooling stages, was developed using a hybrid numerical scheme based on the control-volume/finite-element method in the flow direction, and finite-difference method in the gapwise direction. The theoretical study focused on the determination of polymer/gas interface, residual stresses, and birefringence distributions developed during GAIM. The geometry studied was a tubular cavity in which one-dimensional non-isothermal flow was considered. The viscoelastic behavior of the polymer was described with a non-linear viscoelastic constitutive equation proposed by Leonov [6]. This equation was solved numerically together with mass, momentum, and energy equations using a computer program written in FORTRAN. From the calculated flow-induced residual stresses, the flow-induced birefringence can be determined using the stress-optical rule [7, 8]. The numerical results were compared with the measured birefringence and polymer/gas interface distribution. The experimental part of this study consisted of GAIM experiments carried out in an injection molding machine which has computer-controlled gas-injection and data-acquisition systems. The tubular moldings were obtained by varying the processing
conditions such as: melt and mold temperature, injection velocity, shot size, gas pressure, and gas-delay time. The distribution of the birefringence components $\Delta n$ and $n_{rr} - n_{\theta \theta}$ were measured using a cross polarized microscope and the average birefringence component $<n_{zz} - n_{\theta \theta}>$ was determined using an optical bench.

Thermally-induced stresses, in free-quenched samples and in GAIM moldings, were calculated using a linear viscoelastic theory [9] and the thermally-induced birefringence was calculated with a photoviscoelastic model [10]. These theories were implemented by Shyu [11] for CIM. To consider the change of the polymer density by temperature and pressure, the classical empirical equation of state proposed by Tait [12] was used.

The present work dealt with the two following objectives:

The first was to obtain gas-assisted tubular moldings for two different amorphous polymers under different processing conditions. The processing variables selected were: melt and mold temperatures, gas pressure, shot size, injection speed, and gas-delay time. According to the literature survey, these variables represent the most important parameters that strongly influence the residual wall thickness and gas penetration length in GAIM process. The selected polymers were polystyrene and polycarbonate. Polystyrene has a negative intrinsic birefringence and exhibits a strong rheo-optical effect due to its relatively high stress-optical coefficient in melt state. It has the advantage of being one of the most studied polymers and its birefringence characteristics are amply reported. Because polystyrene has been used by several authors to study birefringence and residual stress distributions in products obtained by different polymer processes, it is especially suitable for data comparison [1, 2, 7]. Besides that, the technique to measure
the polystyrene birefringence is well-established [13]. On the other hand, polycarbonate has positive intrinsic birefringence and it also has a very high stress optical constant. It is a high-performance amorphous polymer frequently used in engineering applications where low levels of residual stresses and birefringence in the final product are generally desirable. Another advantage of using these polymers is that both are transparent, making them suitable for gas penetration observation. To study the influence of the processing conditions on birefringence distribution, measurements of the birefringence components $\Delta n$ and $n_{rr}-n_{\theta\theta}$ and average birefringence $<n_{zz}-n_{\theta\theta}>$ were performed on the tubular moldings. In order to study the influence of thermally-induced stresses in GAIM moldings, free-quenching experiments were conducted in PS and PC tubes and rods at different initial temperatures.

The second objective was to develop a viscoelastic non-isothermal numerical simulation scheme to predict the polymer/gas interface and birefringence distributions in tubular moldings obtained by GAIM. The numerical scheme to solve the governing and constitutive equations together with a set of boundary, initial, dynamic and kinematic interface conditions was based on a hybrid control-volume/finite-element/finite-difference method (CV/FE/FD). The FORTRAN code took into account the viscoelastic behavior of the polymer, by implementing the incompressible viscoelastic constitutive equation proposed by Leonov [6]. The purpose of using a viscoelastic constitutive equation in GAIM was to translate the non-linear rheological behavior of polymeric fluids to computational calculations in order to predict the build-up and stress relaxation of stresses and birefringence that take place during the GAIM process. The flow-induced residual stresses were calculated from the shear stress and the first and second normal
stress difference obtained with the Leonov model. The flow-induced birefringence was calculated using the flow-induced residual stresses profile through the stress-optical rule [8]. Oda, White, and Clark [14] argued on the basis of experiments that the molecular orientation in polymer glasses can be determined using the rheo-optical rule that is valid until polymer reaches the glass transition temperature \( T_g \) where the birefringence becomes frozen-in.

This dissertation is divided into nine chapters. Chapter II presents a background and a literature survey of experimental studies carried out in GAIM. Furthermore, it presents a review of the viscoelastic simulations and birefringence measurements carried out in conventional injection moldings.

Chapter III describes the mathematical derivation to model the GAIM process. The gas penetration was modeled based on the dynamics and kinematics at the interface between the polymer and the gas. The flow-induced stresses were calculated using a nonlinear theory and the flow-induced birefringence was calculated, from the stresses, using the stress-optical rule.

Chapter IV presents the mathematical derivation of the thermally-induced residual stresses and birefringence for free-quenching of tubes and rods. The thermal stresses were calculated using a linear viscoelastic theory considering a cylindrical body that undergoes inhomogeneous temperature variations. The thermally-induced birefringence was calculated from thermal stresses using a photoviscoelastic theory.

Chapter V explains the experimental procedure to obtain the gas-assisted injection moldings, to measure the birefringence components, and to determine the polymer/gas interface distribution.
Chapter VI presents the measurements and simulations the polymer/gas interface
distribution for GAIM experiments at different processing conditions, for the two
polymers employed. It also shows the results of the simulated transient birefringence, $\Delta n$, during filling and gas penetration stages during GAIM. After that, the results of the simulated flow-induced birefringence and measurements of birefringence in GAIM samples, including the simulations and measurements of the average birefringence under different processing conditions. This chapter also shows the measurements of $\Delta n$ and $n_{rr}$, $n_{\theta\theta}$ carried out after annealing a section of a GAIM molding. This chapter concludes with a discussion of the effect of the thickness of the slices isolated from the GAIM moldings to measure the distribution of birefringence.

Chapter VII presents the measured and simulated components of the thermally-induced birefringence and simulated thermal stresses for free-quenched tubes and rods.

Chapter VIII shows the simulated total birefringence for GAIM moldings of polystyrene and polycarbonate. The total birefringence takes into account both the flow- and thermally-induced birefringence. The calculated total birefringence is compared with birefringence measurements.

Chapter IX summarizes the findings of the present study.
CHAPTER II
BACKGROUND AND LITERATURE SURVEY

2.1 Gas-Assisted Injection Molding

The history of the development of the GAIM process was given by Avery [15]. According to this author, the search for the technology to make hollow parts started around 1944 when Opavsky patented a method to inject gas or liquid into a resin. This procedure was performed using a hypodermic needle. However, these early techniques were unsuccessful due to the high pressure developed during the injection molding. One of the preceding techniques to gas-assisted injection molding was the co-injection molding to fabricate articles of synthetic resins with an outer material having a smooth surface and a core of porous material. One of the most notable developers of this technique was Robert Hanning [16,17]. The gas-assisted injection molding technique, as we know it today, was developed in the mid 1970s. One of the pioneers developing this technique was Friederich at Rhom in Germany. In his patent [18], he described a method for injection molding of hollow-shaped bodies made from thermoplastic resins. This process, involves a dynamic interaction of two extremely different materials being injected into the same mold cavity, the polymer and the gas. Essentially the GAIM process consists of three stages: 1) filling, 2) gas penetration, and 3) cooling. In the first stage, the polymer is injected to partially fill a cold mold cavity. The polymer is injected
by a reciprocating screw that transports, melts, and serves as a plunger to pressurize the polymer for injection. The first stage of GAIM is similar to CIM except that it terminates before the cavity is completely filled. In the second stage, which is known as primary gas penetration, pressurized gas is injected either immediately after the first stage has ended or after a certain delay of time between the first and second stages. The compressed gas of controlled pressure or volume is injected into the mold through the nozzle, runner or cavity. The gas takes the path of least resistance to penetrate and hollow out a network of gas channels, forming an advancing round- or bullet-like-shaped bubble which displaces the melt at the hot core to completely fill the cavity. The advancing gas bubble leaves behind a polymer layer at the mold walls yielding a product with a polymer skin and hollow gas channels. In the third stage the gas pressure is maintained to pack the filled cavity while the polymer is cooling down. During this stage, further gas penetration takes place which is known as secondary gas penetration. The secondary gas penetration is caused by the combined effect of the gas pressure and the polymer density change during polymer solidification. In this stage, the gas penetration rate is considerably lower than that of primary gas penetration. Finally, when the part has solidified, the gas is vented and the part is ejected [15, 23]. Outside Germany, the gas-assisted injection molding technique began when foam molders went from producing cellular components to produce parts with large hollow sections in an attempt to overcome surface appearance problems. Companies such as Hoover Universal and KMMCO in the United States and Peerless Foam Molders in the United Kingdom were active in developing the gas-assisted injection molding technique to compliment their structural foam process in order to overcome the surface appearance issues.
Peerless patented its Cinpres I (Controlled Internal Pressure Molding) process in 1993. The process involved injecting a controlled quantity of an inert gas (usually Nitrogen) under pressure, directly into a plastic melt, to form continuous hollow channels throughout the part. Commercial production of moldings using this technique started in 1984. Later, modification to this process were made in order to control more accurately the gas injection pressure profiles introducing Pressure Controllers based on state of the art electro-magnetically operated pressure valves. Around 2001, European companies and machine manufacturers, including Battenfeld, Ferromatic, Stork, Engel, and Johnson Controls, developed variations of this process. Recent developments in gas-assisted injection molding focused on the design of check valves [19,20] and gas injecton pins [21] and control of the process [22].

Some advantages of GAIM in comparison with CIM are: reduction of energy consumption, clamping force and article’s weight, higher stiffness-to-weight ratio in structured parts, improved external appearance and dimensional stability, reduce sink marks and a reduction of flow- and thermally-induced residual stresses [23]. GAIM has some disadvantages, among them are additional cost of inert gas, gas nozzle design, erratic gas penetration in thin sections (fingering effect), uneven gas penetration, air entrapment, hesitation marks on the surface of the molding due to the stop of the melt flow during the polymer-to-gas switch-over, the process leaves a hole in the part where the gas pressure is relieved, multiple cavities are difficult to fill compared to CIM and the introduction of new variables to the process that make it more complicated to control [15, 24]
2.2 Gas Penetration in Fluids

The study of gas bubble penetration in fluids confined in tubes has an important application in GAIM. The early studies on this subject focused on Newtonian fluids [25-27]. Fairbrother and Stubbs [25] performed experiments in a long capillary tube, where a Newtonian liquid flowed at constant rate containing a long air bubble. They compared the true velocity of the liquid measuring its volumetric flow emerging from the capillary tube with its apparent velocity determined with the linear velocity of a long gas bubble traveling inside the capillary tube. They found that when the air bubble penetrated the liquid confined in the capillary tube, it left behind a certain fraction of liquid sticking at the tube wall. They calculated the fractional coverage \( m \), which is defined as the fraction of the tube cross-sectional area coated by the fluid after the gas penetration. The results showed that increasing the bubble linear velocity, the difference between the true and apparent velocities of the fluid is bigger due to an increase in the fractional coverage. It was concluded that the two most important factors on the process are the viscosity and surface tension of the liquid. From the experimental observation, an empirical relationship was established to calculate the fractional coverage, \( m \), as:

\[
m = \sqrt{U_a \mu / \sigma}
\]

(2-1)

where \( U_a \) is the bubble velocity; \( \mu \) is the Newtonian viscosity and \( \sigma \) is the surface tension of the fluid.

Taylor [26] made similar experiments as those carried out by Fairbrother and Stubs using different fluids and capillaries. He found that by plotting the fractional coverage versus capillary number \( (Ca) \) all of the values collapsed onto a master curve
regardless of tube diameter and fluid properties. The capillary number is the ratio of viscous to surface tension forces and is defined as:

\[ Ca = \frac{\mu V}{\sigma} \]  

(2-2)

where \( \mu \) is the Newtonian viscosity, \( V \) is the fluid velocity, and \( \sigma \) is the surface tension.

In addition, Taylor concluded that the fractional coverage reached an asymptotic value of 0.56 when \( Ca > 1.5 \) showing that the empirical relationship found by Fairbrother and Stubbs [25] is valid only when \( 0 < Ca < 0.09 \). Out of this range, Eq. (2-1) overpredicts the fractional coverage. Taylor also proposed how streamlines develop inside the fluid during bubble penetration. Some of these patterns were confirmed by Cox [27] using a photographic technique and tracing particles.

In order to understand the importance of the viscoelastic behavior of polymers on the layer of polymer deposited in the tube wall during gas penetration, Huzyak and Koelling [28] compared the behavior of two Newtonian and two highly elastic (Boger) fluids confined in capillary tubes to determine the effects of the fluid elasticity on the fractional coverage during gas bubble penetration. The experiments were conducted at low Reynolds’ numbers \( (Re) \) and Bond/Capillary ratios \( (10^{-6} < Re < 10^{-3} \text{ and } 10^{-4} < Bo/Ca < 10^{-1}) \) to neglect the contributions of inertia and gravity. The Bond number \( (Bo) \) represents the ratio of gravitational to surface tension forces which is defined as:

\[ Bo = \frac{g(\rho - \rho_f)d^2}{\sigma} \]  

(2-3)

where \( d \) is the bubble diameter, \( g \) is the gravitational acceleration, \( \rho \) and \( \rho_f \) are the bubble and fluid densities, respectively.
The results showed that at low capillary numbers, the fractional coverage of the viscoelastic fluids is nearly identical to that of the Newtonian fluids, showing that the elasticity of the fluids is not important at low shear rates. At high capillary numbers, the viscoelastic fluids deviate from the Newtonian behavior attaining values of fractional coverage up to \( m = 0.73 \), which is considerably higher than the maximum value reported by Taylor [26] for Newtonian fluids. Huzyak and Koelling concluded that the increase in fractional coverage at high strain rate, which corresponds to high capillary numbers, is because of the fluid elasticity. They demonstrated that at low Deborah numbers \((De)\), the value of the fractional coverage for both fluids have a behavior close to that of Newtonian fluids, but when \( De > 1 \) the fractional coverage increases showing that it is dependent on the elastic properties of the fluid. The Deborah number is the ratio of the magnitude of the elastic forces to that of the viscous forces and it is defined as:

\[
De = \frac{\lambda}{t_{\text{flow}}}
\]  

(2-4)

where \( \lambda \) is the polymer characteristic relaxation time and \( t_{\text{flow}} \) is the characteristic time of the flow system.

Gauri and Koelling [29, 30] studied the motion of long bubbles penetrating ideal elastic (Boger) fluids confined in capillary tubes and performed flow field measurements around the leading edge using a Particle Tracking Velocimetry (PTV) technique. They also confirmed experimentally that the fractional coverage deviates from the Newtonian behavior when the Deborah number increases. They also showed that the flow pattern in viscoelastic fluids at low \( Ca \) number is similar to that for Newtonian fluids at the same \( Ca \) number. For high \( Ca \) numbers, a similar pattern was observed as those described by
Taylor [26] and Cox [27]. They also found that fluids with a higher degree of elasticity exhibit a higher fractional coverage than that of the Newtonian fluids.

2.3 Experiments in GAIM

The GAIM of thermoplastics differs from the gas bubble penetration studies because it is a non-isothermal process. This makes the process more complicated because the final thickness of solid polymer deposited on the mold wall, which is known as the Residual Wall Thickness (RWT), is formed by the polymer frozen layer developed during the melt injection stage plus a layer of polymer melt left behind by the advancing gas front during the gas penetration stage [31]. The amount of liquid deposited at the wall during the gas penetration depends on the polymer melt rheology and processing conditions. During the cooling process, the RWT decreases due to the change in polymer density during solidification. Both the gas penetration length and RWT are two important characteristics for the GAIM process and molding quality, because they yield information about the ratio of polymer and gas to be injected into the cavity in the initial stage. If the RWT is thicker than expected, the gas front overtakes the melt front, resulting in what is known as gas breakthrough. When breakthrough happens, the polymer is no longer displaced by the gas and the cavity is not filled completely. The breakthrough can be avoided by injecting a sufficient amount of polymer into the mold cavity prior to the gas injection. The variables which control the GAIM process exert a strong influence not only on the final microstructure but on both RWT and the gas penetration length which define the distribution of the polymer/gas interface of the moldings. Several experimental studies have been done to investigate the influence of the processing conditions of GAIM
on the RWT and gas penetration length. Kapila et al. [32] evaluated the influence of melt and mold temperature, shot size, injection speed, gas pressure and gas-delay time on polycarbonate in a cylinder-shape mold cavity. The analysis focused on part weight reduction, gas penetration length and wall thickness uniformity. From the experiments it was determined that the shot size was the dominating factor for part weight and gas penetration length. On the other hand, the most important factors affecting the RWT were: melt temperature, gas pressure, gas delay time and shot size.

Zhao et al. [33] performed similar experiments with polycarbonate using a single-cavity mold with a center-sprue-gated rectangular plate with a fish-bone semicircular rib layout. They studied the same processing variables as Kapila et al. [32] but held the injection speed constant. It was found that for this geometry, melt temperature, mold temperature and gas pressure do not have significant effects on gas bubble penetration. However, gas bubble length, projected area, gas volume, gas bubble core ratio and gas fingering (an erratic gas penetration behavior) are all dominantly controlled by shot size and gas delay time.

Shin and Isayev [34, 35] studied the effect of the processing parameters on gas penetration in GAIM using standard tensile bar and spiral tube molds. For the tensile bar cavity [34], the injection parameters varied were: shot size, melt and mold temperature, gas-delay time, gas pressure, injection pressure and injection speed. They found that the most influential parameter on the gas penetration length was the melt temperature, followed by the shot size and gas injection pressure, showing the importance of the melt viscosity on the gas injection stage rather than the shot size. In the case of the spiral mold [35], the injection speed was varied in order to investigate the penetration length, residual
wall thickness and melt front position during GAIM at three different temperatures. The results showed that the gas penetration length and RWT decreased when the injection speed was increased. It was concluded that the injection speed exerts a strong influence on both gas penetration and the RWT, and they proposed that injection speed can be used as an alternative to control the RWT instead of gas-delay time. The delay time has the disadvantage of polymer solidification in the sprue when the time is too long.

Jong et al. [36] studied the influence of mold and melt temperature, gas pressure, gas-delay time, gas injection time, and shot size on gas penetration length, size of the gas channels, and wall thickness in GAIM moldings. They used a planar cavity with fishbone semicircular layouts, in which, the gap between the plates and the radius of the ribs were varied. It was found that both, injection time of gas and mold temperature have little influence on the gas penetration length. They also observed that longer gas-delay times yields smaller gas channel cross sections with longer gas penetration. Furthermore, the results showed that high melt temperatures gave long gas penetration and low melt temperatures required higher gas pressure to penetrate. The shot size was found to be the most critical processing parameter for this mold geometry because it was observed that a reduction in the shot size caused either, diffusion of the gas (fingering effect) or breakthrough in the part.

Chen et al. [37] performed an experimental study to investigate the influence of gas pressure, melt and mold temperature, and gas-delay time on the gas penetration length and RWT for polystyrene spiral moldings. They found that the RWT increases with gas-delay time due to the cooling of the melt. Likewise, lower melt and mold temperatures will result in a thicker RWT and, as a consequence, longer gas penetration
length. Furthermore, it was found that the gas penetration decreases when the gas pressure was increased. Chen et al. observed that at low gas pressures and longer delay times, the gas bubble distribution in the moldings showed a gas bulge at the end of the primary gas penetration which indicates the existence of a secondary fountain flow at the gas front. But, at higher gas pressures and short gas-delay times, the gas bulge disappears and the gas penetration shows a smooth transition between the primary and secondary gas penetration.

From literature it is realized that the most influential factor affecting RWT and gas penetration length may be different for each case. It appears that the most influential factor depends on the mold geometry making it difficult to generalize a processing control guide for GAIM process. However, it was observed that the most important variables in the GAIM process are melt injection speed, mold and melt temperature, gas pressure, shot size, and gas-delay time.

2.4 Simulation in GAIM

Experimental studies in GAIM, have shown that the ample variety of mold geometries, polymeric materials and considerable number of processing variables makes it difficult to predict a priori the RWT and gas penetration length for a specific geometry. Thus, computer simulation is required to assist in product and mold design to evaluate the processing window and predict the physical properties of the final product. Simulation in GAIM represents a challenging problem because the polymer/gas interface and flow front represents a moving boundary problem. In spite of today’s remarkable technological progress in computer aided engineering and design (CAE and CAD), mold design
engineers still have problems to designing molds that yield products free of shrinkage, warpage, sink marks, residual stresses and birefringence which are the more challenging problems in injection molding process. For the past two decades, many researchers have modeled the GAIM process using different approaches [38-52]. Polynkin et al. [38] performed experiments and computer simulation using a finite-element method, to investigate the gas displacement of a shear thinning power law liquid in a cylindrical tube under isothermal conditions. The experiments were carried out either at constant gas pressure or at constant gas volume in the range of power law index of $0.1 \leq n \leq 1$ and Reynolds numbers of $0.001 \leq Re \leq 100$. Furthermore, due to the high viscosity of the liquid and high capillary number during the experiments, the surface tension and gravity effects were omitted. The viscosity was modeled using a truncated form of power law and the polymer/gas interface was tracked with the advection equation. The experiments and numerical results showed that the fractional coverage diminishes when the degree of shear thinning and Reynolds number increase. Nevertheless, in the low end of the Reynolds scale, which is relevant for polymer melts, the Reynolds number effect on the fractional coverage is negligible.

Haagh et al. [39] simulated the gas penetration in an incompressible isothermal Newtonian fluid using a pseudo-concentration method with a fixed grid that covers the entire mold. In this method a fictitious fluid is introduced to represent the penetrating gas and the air downstream of the flow front. The two important characteristics of the fictitious fluid are: 1) its viscosity is on the order of $10^{-3}$ of the polymer viscosity, and 2) its density is equal to that of air. In this case the Reynolds number remains low and the pressure drop of the fictitious fluid is negligible compared with that of the polymer melt.
The equation to describe the polymer/gas interface evolution is given by the advection equation. It was demonstrated that the numerical method described with good approximation the experimental results for several two- and three-dimensional geometries.

Potente and Hansen [40] performed numerical simulations and experiments with a PC/ABS blend using a center gated commercial mold with a T-shape cross sectional area. The simulations were carried out with a program developed by Wang et al. [41] based on a hybrid finite-element/finite-difference/control-volume scheme which used C-MOLD™ application to generate the mesh. The authors analyzed the influence of gas-delay time, mold temperature, and shot size on the fractional coverage. The generalized Hele-Shaw flow approximation was used to describe the inelastic, non-Newtonian flow under non-isothermal conditions and the polymer viscosity was described using the 5-constant Cross-exponential model. They state that the simulation results agreed very well with the tendencies found in the experiments, showing that the most influential parameter in the gas penetration length was the shot size, followed by the gas-delay time. Also, they found that the mold temperature results in thicker RWT in the molded part.

As stated before in Section 2.1, primary and secondary gas penetrations result from two different mechanisms. The former is caused by the displacement of the molten polymer by the pressurized gas while the latter has its origin in the polymer melt shrinkage during the cooling process. The secondary gas penetration has been taken into account in numerical calculations of GAIM by several authors [42-52]. Chen et al. [42-46] carried out numerical simulations and experimental studies on both a thin plate with a semicircular gas channel and spiral tube molds. The algorithm was based on a hybrid
control-volume/finite-element method that takes into consideration both primary and secondary gas penetration in an inelastic, non-Newtonian fluid under non-isothermal conditions. The non-Newtonian polymer melt viscosity was described by a modified Cross model with Arrhenius temperature dependence. The calculation of the secondary gas penetration was based on the melt shrinkage and compressibility of the polymer melt governed by the P-V-T equation of state originally proposed by Tait. To calculate the pressure field during the melt injection stage, the governing equations were discretized using a standard Galerkin finite-element method. The numerical scheme provides reasonably good results in the prediction of primary and secondary gas penetration. The advancement of both melt and gas fronts in a spiral tube mold of circular cross section were also simulated using the previous scheme [43]. Although no effect of processing conditions was investigated, the experimental observation of the primary and secondary gas penetrations were consistent with simulations. Chen et al. [44, 45] extended this approach to simulate the gas penetration in a thick hanger and thin angle bracket plate with gas channels of quadrantal cross section. The numerical results coincided reasonably well with measurements. In Ref. [46] Chen et al. studied the influence of melt temperature, injection speed, mold temperature, gas-delay time, gas pressure, gas-injection and holding time, and shot size on gas penetration length and RWT in a single-hanger mold geometry. The results showed that the frozen layer thickness is very sensitive to polymer melt temperature, injection speed and mold temperature. Increasing the gas pressure and holding time increases the secondary gas penetration during packing stage. Although numerical simulations showed good tendency for the gas flow, there is still discrepancy between the experimental and simulation results.
Barton and Turng [47] and Turng [48] studied the effect of processing variables and presented a general design guideline for GAIM using CAE analysis. They found that the variables that have more significant impact on the process are: gas pressure, gas-delay time, melt temperature, shot size, and gas injection time. However, they stated that in spite of the guidelines for designing the GAIM molds, it is difficult to determine the best combination of variables to optimize the process.

Li et al. [49, 50] performed experiments and simulation to describe the polymer/gas interface distribution developed during the primary and secondary gas penetration in a non-isothermal GAIM process. They investigated the influence of processing variables such as: melt temperature, shot size, gas pressure, injection speed, and gas-delay time using a spiral mold with circular cross sectional area. A hybrid method based on control-volume/finite-element/finite-difference was implemented to discretize the equations for both the fluid and gas domains. A finite-element method in the flow direction and a standard finite-difference technique in the gapwise direction and time were employed. To keep track of the polymer/gas interface, time dependent kinematics of the interface evolution equation were used and the viscosity was described by the four-parameter Cross model. The predictions of the model were compared with experimental results and with simulations performed with the commercial package C-MOLD™. Good agreement was found between the numerical results and experiments. Shot size was found to have the strongest effect on gas penetration length, while injection speed and gas delay time have a significant effect on RWT. The numerical results obtained with the developed code were found to be more accurate than that of C-MOLD™.
Polynkin et al. [51] implemented a three-dimensional finite-element code for the simulation of GAIM of a handle with circular cross-sectional area. They studied the cooling effect on the primary gas penetration and RWT by varying the gas-delay time. The computer code for a non-isothermal process was based on the pseudo-concentration method and the non-Newtonian viscosity data was fitted using the Cross model. Although the code developed by Polynkin can predict the secondary gas penetration, this effect was not included because it was found to be negligible for the geometry analyzed. The results obtained with this method showed excellent predictions including the increase of the RWT due to cooling when the gas delay time was increased.

Recently, Polynkin et al. [52] developed a relatively cheap short cut method based on finite elements to predict the polymer/gas interface distribution in GAIM considering a generalized Newtonian fluid flow. The method is based on the solution of a steady single phase flow of the polymer melt filling the cavity of interest. The polymer/gas interface is approximated by introducing an appropriately defined mean velocity which is computed by integrating the flow velocity normal to the cross section and dividing it by the adjusted cross-sectional area. The adjusted cross-sectional area is obtained by adding finite-element areas where the mean normal velocity is greater than or equal to the empirically-specified fraction of the maximum velocity on the cross section. The results were found to be in good agreement with experiments. However, it was found that for complex geometries, full analysis of the polymer/gas flow dynamics is required.
2.5 Residual Stresses and Birefringence

Residual stresses play an important role in the final properties of polymeric products [1,2,5]. In injection molding and other polymer processing operations, the polymer experiences different thermo-mechanical histories depending on the processing conditions. High stresses and fast cooling, typically encountered in most of the polymer processing operations, leads to molecular orientation and, as a consequence, residuals stresses are developed in plastic products. Molecular orientation renders optical and mechanical anisotropies as well as dimensional variations. Residual stresses and birefringence in polymeric parts have been widely studied for many years. The increasing demand of polymeric products for special applications, such as optical [23, 53] and medical [54] devices, which require low levels of birefringence and residual stresses, makes the study of birefringence and residual stresses a topic of current interest in polymer processing; especially in those processes where the flowing polymer melt experiences high level of stresses and a fast cooling. Almost all polymer processing operations exert high stresses to the polymer melts and tend to align the molecules in the flow direction. This effect, in combination with cooling leaves frozen-in molecular orientation when the plastic solidifies leading to anisotropy of the properties of the plastic parts.

Frozen-in orientation and residual stresses in the injection molding of amorphous polymers appear from two main sources [2]. The first one is the flow-induced stresses (shear and normal stresses), developed in the polymer melt during the filling of the mold cavity. These stresses cause molecular orientation that, during the subsequent cooling stage, do not relax completely and the molecules remain oriented causing frozen-in
birefringence and flow-induced residual stresses in the molded part. The second source of residual stresses and birefringence is due to the combined effect of the non-equilibrium density change and the viscoelastic behavior of the polymer that takes place during the inhomogeneous rapid cooling through the glass transition temperature \(T_g\) which results in thermally-induced residual stresses and birefringence.

Thermally-induced residual stresses due to rapid change in temperature were observed in inorganic glasses. Aggarwala and Saibel [55] calculated the residual stresses in plates using the instant freezing assumption, originally proposed by Bartenev [56, 57], considering that above a certain critical temperature glass behaves like inviscid compressible liquid and below this temperature the glass behaves like elastic solid.

Wales [58] performed birefringence measurements on polymers melts flowing under a high shear stress through a slit die. He has shown that the flow birefringence \(\Delta n\) of polystyrene melt is related to the shear stress at the wall. Lodge [59] derived rheological and optical equations of state and showed that, for flowing polymer solutions, the refractive index ellipsoid and the stress ellipsoid have the same orientation, and that their components are proportional to each other. The measurement of flow birefringence can be used to determine molecular orientation and stress tensor via a relationship known as the stress-optical rule [8]. The linearity of the stress-optical rule is valid for stresses up \(10^6\) Pa [8].

One of the pioneering studies on residual stress in polystyrene injection moldings was performed by Spencer and Gilmore [1]. They described the fluid dynamics during the mold filling and discussed the origin of three different types of residual stresses: 1) quenching; 2) frozen-in molecular orientation; and 3) configurational volume strains.
Thermally-induced residual stresses arise during the cooling process, in which the molecules are drawn close together and their configuration becomes more compact causing inhomogeneous density variations through the sample thickness. The frozen-in molecular orientation has its origin in the high elasticity attributed to the uncoiling of normally coiled-up polymer molecules which, during the deformation, tend to align in the flow direction. As a polymer is cooled through the softening point the molecular chains become less and less mobile and, if the softening point is reached while the stress is still acting, the molecules become frozen in the uncoiled state and remain oriented in the polymeric part. The residual stresses caused by the configurational volume strains, which are due to changes in molecular configuration while the polymer is cooling, are considered insignificant and unimportant for practical cases.

Wimberger-Friedl [60-62] performed experimental studies on birefringence distribution, parallel \((n_{yy}-n_{zz})\) and perpendicular \((\Delta n)\) to the flow, on polycarbonate flat plates and compact discs obtained by injection molding under different processing conditions. For both the flat plate and disc moldings [60], the birefringence distribution \(\Delta n\) shows a classical maximum at the surface which depends on the filling and packing conditions as shown by Isayev [2]. In Ref. [61] the author stated that the maximum birefringence is caused by the frozen-in elongational orientation built up in the fountain flow of the advancing front, flow-induced orientation and cooling stresses. It was found that the thickness of the solidified layer formed during the filling stage depends on the injection speed and mold temperature. The birefringence \(\Delta n\) at the core is highly influenced by the processing conditions especially by packing pressure and melt injection velocity. In Ref. [62], Wimberger-Friedl compared the birefringence in injection molding
flat plates with that developed in constrained quenched plates. The injection moldings were obtained at high melt injection speed and no packing pressure. It was found that the birefringence in the core of the injection molding plates is almost identical to that of the quenched samples, as shown earlier by Isayev [2]. This shows that shear stresses can be confined in the frozen-layer and the birefringence at the core is caused by quenching effects.

A lot of effort has been put forth to predict the birefringence components and frozen-in orientation in injection molded parts. One of the pioneering works to predict frozen-in orientation was carried out by Tadmor [63], who proposed a semiquantitative model based on molecular theories (bead-spring model derived by Bird et al. [64]) in elongational and shear flow coupled with flow and heat transfer mechanisms, to explain the complex molecular orientation distribution observed in injection moldings of amorphous polymers. He found that both the orientation in the close neighborhood of the wall and the transverse orientation originate from the fountain type flow in the advancing front region whereas the source of the rest of the orientation is primarily from the shear flow upstream the front.

Kamal and Tan [65] performed theoretical and experimental studies of the distribution of the birefringence components $\Delta n$ and $n_{yy} - n_{zz}$ along the wall thickness of molded strips by considering the actual pressure time cycle of the molding operation and the stress-optical relationship. The results show that the maximum birefringence of both $\Delta n$ and $n_{yy} - n_{zz}$ are attained at the wall and it decreases towards the center of the molding. Theoretical and experimental results of birefringence component $\Delta n$ were compared using the expression proposed by Wales [58]. This expression relates the birefringence
component $\Delta n$ with shear stress at the wall. The theoretical results show good agreement with experimental ones. But it seems that mathematical expression proposed by Wales [58] cannot predict the birefringence component $n_{yy} - n_{zz}$.

Wales [66] compared the birefringence of injection molding plates and the birefringence during steady isothermal shear flow in a slit die. He found that the average value of the birefringence during the steady flow, $<n_{xx} - n_{zz}>$, is a function of the squared shear stress at the wall. Also, it was shown that the anisotropy induced by flow is governed by the shear stress regardless of the temperature. The average birefringence $<n_{xx} - n_{zz}>$ patterns of injection molding show small deviations from those for steady isothermal flow. The birefringence $\Delta n$ for the injected plates shows a maximum at the wall with a steady decrease towards the center. For the isothermal flow, it is expected that a birefringence maximum occurs at the channel walls with a steady decrease to zero at the channel center.

Janeschitz-Kriegl [67] presented a theoretical analysis to explain the birefringence distribution of $\Delta n$ and average birefringence $<n_{xx} - n_{zz}>$ through the thickness and along the length of flat injection moldings, respectively. Using the experimental data of Wales [66], He developed an analytical thermal model which describes the growth of the solidified layer of the polymeric part as a function of time during the injection molding process for any distance from the injection gate. The power-law model was used to determine the stress tensor and the rheo-optics method was applied to predict the behavior of the molecular orientation and birefringence. The maximum peak observed in the distribution of birefringence $\Delta n$ through the thickness of the part, was explained based on the increase of shear stress due to the reduction in cavity height caused by the growing of the
solidified layer during the non-isothermal filling stage. So the distance of the maximum peak of $\Delta n$ from the wall corresponds to the thickness of the solidified layer at the end of the filling stage. On the other hand, measurements of average birefringence $<n_{xx} - n_{zz}>$ show a maximum located at the same distance from the sprue where the channel has its minimum height and, as a consequence, maximum shear stresses during the mold filling.

White and Dietz [7] predicted the birefringence distribution of $\Delta n$ component along the thickness direction of strip injection molded parts. They used an empirical correlation between the first normal difference $N_1$ and shear stress $\sigma_{xy}$ given by the second order fluid and the empirical correlation of Oda, White, and Clark [14] and the stress-optical rule. The measured birefringence profile along the thickness direction shows a minimum value at the center of the cross section and a maximum at about seventy percent of the distance to the mold wall. $\Delta n$ decreases, then passes through a minimum and rises again to exhibit a second maximum at the mold wall. The theoretical results show a reasonable agreement with the experimental ones.

2.6 Rheological Models

The Newtonian constitutive equation is the simplest model to describe the viscosity of a fluid in which the viscosity is the proportionality constant between the deviatoric stress and deviatoric rate of strain tensors. The range of validity of the Newtonian constitutive equations is limited to fluids, in which the viscosity is independent of the shear rate, called Newtonian fluids. Due to the viscoelastic nature of polymeric fluids, they exhibit a different flow behavior than that of Newtonian fluids. They exhibit some peculiar phenomena such as: rod-climbing, extrudate swell, tubeless
siphon, viscosity shear-rate dependence (shear thinning), normal stresses differences and memory effects associated with the elasticity of the material [68, 69]. A Newtonian model cannot predict the flow phenomena observed in polymeric fluids. In general, constitutive equations should yield predictions of stresses and strains generated during the material flow and they should be based on ideas that do not contradict physical principles. The fundamental difficulty in predicting the properties of the polymeric materials is its nonlinear behavior observed in steady and dynamic flow regimes. Rheological constitutive equations contain material-dependent properties needed to determine macroscopic transport of fluids. Except for Newtonian fluids which obey a linear law, rheological constitutive equations are almost always nonlinear. It is worth mentioning that some pure viscous models such as generalized Newtonian fluid, the power-law model, the Ellis model, Carreau-Yasuda model, and the modified Cross model can describe the shear thinning behavior of the polymer melts. An excellent review of these models can be found elsewhere [68-70]. One of the most popular models is the power-law constitutive equation. It is a well known and widely used empiricism because the algebraic simplicity and the small number of material parameters make it attractive for engineering calculations. The most serious limitation is that this model can not predict the viscosity at very low shear rates [68]. There are some other models such as Carreau-Yasuda and modified Cross models [68, 70], which due to their flexibility to fit a wide variety of experimental viscosity curves, are used in numerical calculations. One of the serious drawbacks of pure viscous models is that they cannot predict stress relaxation effects and memory effects which are one of the main characteristics of polymeric fluids. In these models stresses become zero as soon as flow ceases.
A significant effort has been put forth to obtain constitutive equations capable of describing the strongly nonlinear behavior of the polymer melts and solutions at high Deborah numbers. Many rheological equations have been developed which have the ability to describe transient and relaxation phenomena in standard simple shear and extensional flows within the limited region of deformation rates employed in rheometric tests. The problem is that in real processing operations, the values of the Deborah number (De) may be at least two orders of magnitude higher than in usual standard rheological tests. Extrapolation of these equations to the region of high Deborah numbers results in instabilities [71-67]. Leonov [72], and Kwon and Leonov [73] stated that there are two types of instabilities in constitutive equations: Hadamard and dissipative. A Hadamard instability is a non-evolutionary character of the set of governing equations, which results in a progressive failure of numerical calculations. A complete set of equations for viscoelastic liquids is Hadamard stable when its solution at any time, provides the complete initial conditions for determining the solution at subsequent instants in time. Thus, the calculation progresses in the positive direction of the time axis. A dissipative instability is due to inappropriate modeling of the dissipative term in the constitutive equation. It can occur even if the dissipation term is positive definite. Dissipative instability is manifested as the unboundedness of constitutive equations and is related to the improper formulation of the dissipative terms in the evolution equations.

Viscoelastic models can be divided into two categories: integral and differential type. For simulation, integral type models are not widely used because it is necessary to declare large arrays to store the stress or strain histories. However, one of the advantages of some integral models is that they are explicit in the stress. In flow simulations this
means that the stress components can be eliminated and the total number of dependent variables may be reduced. However, if the stress is included in the memory function this elimination is no longer possible [68].

From the differential type models, the constitutive equations proposed by White-Metzner, Leonov, and Giesekus have been widely used in simulation. The White-Metzner model [74], has the advantage of being relatively simple and gives reasonable predictions for the shear-rate dependent viscosity and first normal stress coefficient. This model has been successfully used in computer simulations for different flows: two-dimensional contraction [75], and in injection molding [76, 77]. The Leonov model [6] is derived using a quasi-linear irreversible thermodynamic approach with the recoverable strain tensor considered as an internal parameter. In Leonov’s formulation, the stored elastic strain is allowed to dissipate by a non-equilibrium process known as a relaxation [69]. The Leonov model has been used quite successfully to predict the viscoelastic behavior of polymer melts. The Giesekus model is based on anisotropic drag created by the oriented molecules during the flow. It was derived for concentrated solutions and melts by starting from the dumbbell theory for dilute solutions [69]. This model predicts well the steady-state shear viscosity, first and second normal stress difference, and stress relaxation in different types of flow [69, 78].

Upadhyay and Isayev [79, 80], Isayev and Hieber [81], and Simhambhatla and Leonov [82] have modeled different types of flows of polymer melts using a highly nonlinear specification of the general class of Maxwell-type constitutive equation proposed by Leonov [6]. The set of governing equations were specified within the global stability constraints to be Hadamard and dissipative stable. The numerical results were
compared with available experimental data, showing a good description for a large variety of rheometric tests.

Kwon and Leonov [83] studied Hadamard and dissipative type instabilities of various factorable single integral constitutive equations, concluding that there is no viscoelastic single-integral constitutive equation of factorable type proposed in the literature, that could satisfy all the stability criteria for Hadamard and dissipative stability.

As a result of Leonov’s analysis only the Finitely-Extensible Nonlinear Elastic (FENE) and Leonov models are globally Hadamard and dissipative stable and the Upper Convected Phan-Thien-Tanner model is Hadamard stable but dissipative stability depends on dissipative terms.

Kwon and Leonov [83] found that none of the specifications of the single integral constitutive equations are globally stable. However, there are four globally stable specifications of the differential type: the FENE dumbbell model, the upper convected Pan-Thien-Tanner (PTT) model, the Giesekus model with a generalized elastic potential, and the stable general class of the Leonov constitutive equations.

The major advantage of using the constitutive Leonov constitutive equation is its firm foundation on non-equilibrium thermodynamics that consequently has resulted in global mathematical stability.

Great efforts have been made in the development of simulation techniques in different polymer processing operations of polymers. A good review of these techniques are given by Isayev [84] and Tucker [85]. The rheology of the polymer melt has been modeled using inelastic models with shear-rate and temperature-dependent viscosity functions. However, these models can not predict normal stresses originated during the
flow, residual stresses or frozen-in molecular orientation in molded products. In order to model these stresses, viscoelastic models have to be included in simulations.

2.7 Viscoelastic Simulations

One of the ultimate goals of numerical simulation in polymer processing operations is to render the mechanical and optical properties of the final product based on the material properties and the processing conditions. As indicated in the previous section, pure viscous constitutive equations for polymers are good enough to analyze the process but not to predict the final properties of the product. The use of different constitutive equations to simulate the time-dependent nonlinear flow behavior of polymer melts has been reported by several authors. Larson [86] compared the numerical results of two models with experimental data for homogeneous elongational flow. The two models employed are: the Wagner model [87, 88] which is a single integral type constitutive equation and the Leonov model [6] which is a differential type constitutive equation. He found that the Wagner constitutive equation can predict quantitatively the experimental data but it has the disadvantage of being difficult to handle numerically. The Leonov model is not quite accurate in elongational flow, but quantitative agreement can be obtained by adjusting empirically the nonequilibrium potential. This can be done by making each relaxation time dependent upon the recoverable strain. Also the Leonov model has the advantage of having a simple differential form which, in numerical calculations, can be implemented without difficulty.

Some constitutive equations work well for a certain shear rate interval. For example, Yen and McIntire [89] tested the integral type Bernstein-Kearsley-Zapas (BKZ)
fluid model [90], determining the strain energy function from small-amplitude oscillatory shearing data. The author suggested that the BKZ fluid model can be used only for moderate shear rates.

Upadhyay et al. [91] performed numerical simulations using the multi-mode Leonov constitutive equation for a wide range of elastic strains for three time-dependent problems: i) stress growth after suddenly applied constant shear rate and the relaxation after the flow cessation; ii) the stress relaxation after suddenly imposing a constant shear strain; and iii) the elastic recovery after shear flow. The authors pointed out that the practical advantage of the Leonov model is that the model parameters can be calculated from either experimentally determined storage and loss modulus versus frequency or from steady-state shear viscosity and first normal stress difference data. The predicted results of birefringence and extinction angle based on the Leonov model are found to compare well with the experimental data for both polymer melts and solutions.

Leonov and Prokunin [92] improved the Leonov model [6] using the empirical Blatz-Sharda-Tshoegl (BST) elastic potential. They tested the new model for simple shear and extension flows finding that by using the BST elastic potential function, the results are described more accurately.

Due to the viscoelastic nature of the polymer melts and its influence on the stress development during processing, attention has been paid to the effect of viscoelasticity on the numerical simulation of final residual stresses and birefringence in polymeric parts. One of the pioneering works in birefringence determination using viscoelastic numerical simulations was performed by Isayev and Hieber [81] who made theoretical calculations of residual stresses, molecular orientation and three components of birefringence $\Delta n, n_{zz},$
and the average birefringence \(<n_{xx} - n_{zz}\>). The calculations were made considering an idealized problem in a Poiseuille-type flow between parallel plates using a finite-difference scheme. They use the viscoelastic constitutive equation proposed by Leonov [6] with two relaxation modes coupled with the governing equations for non-isothermal flow in both filling and cooling stages. The theoretical calculations were compared with injection molding experimental data available in the literature by Wales [66, 93], Janeschitz-Kriegl [67] and Kamal et al. [94], showing in many respects a good correlation.

Isayev [2] also performed experimental measurements and calculation of birefringence on freely and constrained quenched strips and injection molded parts made of polystyrene (PS) and poly(methyl methacrylate) (PMMA). The injection molding experiments were carried out using different processing conditions. It was found that the birefringence perpendicular to the surface of the free quenched plates of PS is zero. This indicates that the birefringences through the thickness in the two other planes of the plate are equal. Furthermore, the birefringence distribution through the thickness showed a parabolic shape with positive and negative values near the surface and cores regions, respectively. The birefringence distribution in the free quenched samples of PMMA showed that the positive birefringence in the core region that relaxes at long times while the negative birefringence near the surface does not relax. This phenomenon was not observed in PS samples. The sign reversal between the distributions of birefringence in the free quenched samples of PS and PMMA was attributed to the stress optical coefficient (C) of these two polymers. The value of C for PS is negative and positive above and below \(T_g\), respectively, while the value of C for PMMA is positive and
negative below and above $T_g$. For PS quenched samples, the thermally-induced birefringence distributions of free and constrained quenched strips are totally different. In the PS freely quenched samples the birefringence showed a change in sign, positive in the center and negative near the surface. For the constrained quenched samples, the birefringence turns out to be negative throughout the thickness. In the case of PMMA quenched samples this phenomenon was not observed. On the other hand, the final birefringence in the injection molded parts is a result of the coupled effects of flow- and thermally-induced molecular orientation. Comparison between the experimental results and the theory introduced in Ref. [81] shows that the calculations predicts a zero value of birefringence at the center while the birefringence measurements show a non-zero value along the thickness with a maximum near the wall. In spite of the zero birefringence prediction at the center, the calculated birefringence near the wall is in good agreement with the measurements. The author claims that the zero birefringence prediction at the center is because the calculations do not take into account the thermally-induced birefringence.

Shyu et al. [95] developed a numerical simulation program using a finite-element method for the injection molding of a center-gated disk, considering filling, packing and cooling stages. The viscoelastic constitutive equation developed by Leonov [6] was used for stress calculation. To consider the volume change during cooling, the PVT relationship was assumed to follow the Tait equation. The flow induced birefringence was related to the flow stresses calculation performed using the viscoelastic constitutive equation through the linear stress-optical rule [8]. Predicted gapwise distribution of birefringence $\Delta n$ and average birefringence $<n_{\theta}\tau n_{\theta}>$ at various radial positions with and
without packing are compared with experimental results by Yoon [96]. The numerical results are in good agreement with the experiments reported, except for the zero birefringence predicted at the center of the moldings. Experimental data indicates that there is certain degree of birefringence at the center. The possible reason for the difference is thermally-induced residual stress built up in the molded disk including the centerline of the cavity as shown by Isayev [2].

As a consequence of the birefringence effect, which accompanies molecular orientation, the use of transparent plastics for optical applications is very much restricted. Molecular orientation is not only introduced during the filling, but also during the post-filling (packing and holding stages) of injection molding process.

Baaijens [97] simulated the flow- and thermally-induced residual stresses developed during filling and post-filling stage in 2D injection molded parts. He modified the traditional incompressible Leonov model to include compressibility effects, performing a kinematic split of the elastic deformation tensor into a volumetric and a deviatoric part. To calculate the flow-induced residual stresses two approaches were developed. In the first method, the melt flow problem is formulated using the viscoelastic model. In the second, the melt flow problem is formulated assuming a generalized Newtonian material behavior, and the resulting velocity and shear rate fields are used to calculate the normal stresses employing the compressible Leonov model. He found that the second technique gives similar results to the first one and the computational cost is significantly reduced. To calculate the thermally-induced residual stresses, Baaijens employed the linearized Leonov model, which reduces to the Maxwell model.
Flaman [98] developed a numerical simulation model for the analysis of the buildup and the relaxation of molecular orientation and frozen-in birefringence $\Delta n$ in injection molded products using an extended version of the multi-mode Leonov model. Compressibility in the Leonov model was introduced by kinematic split of the elastic deformation tensor as done by Baaijens [97]. The frozen-in birefringence is coupled with stresses through the stress-optical rule, and it was calculated for different processing conditions. The results show that, among the four processing parameters evaluated, the flow rate has a major effect on the frozen-in birefringence while the second most important parameter is the melt temperature. The effect of the mold temperature on $\Delta n$ is not very pronounced and the packing pressure exhibits only a minor effect.

Morland and Lee [9] performed a linear thermo-viscoelastic stress analysis for materials with temperature dependent characteristics on the basis of temperature-time equivalence hypothesis originally proposed by Leaderman [99]. According to Leaderman’s theory, the relaxation moduli and creep compliances in shear and dilatation are affected by a constant temperature change only within a corresponding uniform shift of the logarithmic time scale. The materials that exhibit such a behavior have been termed as “thermo-rheologically simple materials” by Schwarzl and Staverman [100].

Another effect of the viscoelasticity of polymers on its optical behavior is the change of the stress- and strain-optical coefficients with time. This effect has been observed in creep and stress relaxation experiments [101] and it has been included in numerical calculations to predict the thermally-induced residual stresses.

Williams and Arenz [10] described the interrelation between the stress- and strain-optical coefficients and performed an extensive analysis of photoviscoelasticity for
linear viscoelastic materials assuming that the time-temperature superposition principle can be applied to both the mechanical and optical properties of the polymer. They also studied the mechanical and optical properties of a low-modulus polyurethane at constant-strain-rate, finding that these properties are adequately represented by the WLF equation.

Shyu et al. [102] performed tensile stress-relaxation experiments with simultaneous measurements of Young’s modulus and the strain-optical coefficient $C_\varepsilon$ over a wide range of temperatures and times. Master curves of Young’s modulus and strain-optical coefficient for polystyrene and polycarbonate were obtained via time-temperature superposition principle. They found that the strain-optical coefficient $C_\varepsilon$ for polystyrene is positive in the glassy state at low temperature and time. Then, $C_\varepsilon$ relaxes and becomes negative and passes through a minimum in the transition zone from the glassy to rubbery state at an intermediate temperature and time and then increases with time approaching zero at large time. On the other hand, the strain-optical coefficient for polycarbonate is always positive being constant in the glassy state and continues relaxing with time towards zero.

Lee et al. [103] performed numerical simulation and experimental analysis to predict both flow- and thermally-induced residual stresses and birefringence on polystyrene center gated disks obtained by injection molding. For description of the flow-induced phenomena, the Leonov model and stress-optical rule were used. To predict thermal induced phenomena, the linear viscoelastic model, photoviscoelastic model and free volume theory, which takes into account the density relaxation phenomena, were employed as proposed by Shyu and Isayev [104]. Using this scheme, Lee [105] performed numerical analysis to investigate the processing conditions influence on the
final residual stresses and birefringence in injection/compression and injection moldings. The results show that high melt temperature reduces the birefringence in both at the wall and core. As the packing time and packing pressure increase, the birefringence at the core increases significantly, while the birefringence near the wall increases only slightly. The stresses at the surface increase with the packing time and packing pressure. Also, as mold wall temperature decreases, the magnitude of tensile stress at the core layer and the compressive stresses at the intermediate layer increases significantly.

The theory proposed by Janeschitz-Kriegl [67] states that the flow birefringence peak near the molding surface is caused by the shear stresses increment due to the solidified layer growing during the filling stage. Also, the flow birefringence shows a second peak in the core caused by the normal stress difference developed during the additional flow in the packing stage. The radial dependence of the gapwise-average birefringence shows a monotonously decreasing function of radial position. However, when no packing pressure is applied, the flow birefringence shows a zero value at the center while the experimental result indicates certain level of birefringence with a plateau towards the center. This phenomenon is attributed to the thermally-induced residual stress build-up during the polymer solidification. This phenomena has been addressed by some authors using different approaches [13, 97, 98, 106, 107]. Titomanlio et al. [106] proposed a model to calculate the thermally-induced residual stress distribution build-up in rectangular injection moldings. The model takes into account the effect of the interaction of the polymer with the mold and pressure history in the melt during the cooling process. The thermally-induced residual stress distribution through the thickness is related to the strain experienced by the different solid layers that result from the
unidirectional transient polymer solidification. The major simplifications of this model are that the Young’s modulus of the solid polymer and the thermal expansion coefficient are constants. In spite of those simplifications, the model predictions compare fairly well with available experimental data. This model totally neglects the viscoelasticity of the polymer melt and time-temperature-dependence of the polymer near the glass transition temperature.

Struik [107] studied the flow- and thermally-induced residual stresses in injection molding thermoplastic parts. The flow-induced residual stresses were modeled considering that the external and entropic stresses are at equilibrium and the molecular orientation and the entropic stresses become frozen-in when the temperature drops below $T_g$. To calculate the strain produced by the entropic stresses, Struik employed a time- and temperature-independent Young’s modulus formulation. To calculate the thermally-induced residual stresses in polymers with any geometry, Struik generalized the theory developed for quenched inorganic flat glass plates by Aggarwala and Saibel [55], neglecting the viscoelasticity and volume relaxation effect of the polymer during the cooling stage. However, the author acknowledges that the viscoelastic effects and temperature dependence of modulus and thermal expansion coefficient cannot be neglected especially in the glassy state.

Famili and Isayev [84] and Shyu and Isayev [104] performed numerical simulation to calculate the residual stresses and birefringence in center-gated disks made of polystyrene and polycarbonate. The numerical calculations for filling, packing and cooling stages were based on the under-relaxation iteration method reported by Sobhanie and Isayev [108]. Due to the fact that, at the present, there is no constitutive equation able
to describe the rheological behavior of the polymer in both solid and melt states, the flow- and thermally-induced residual stresses were calculated using the Leonov model and linear viscoelasticity, respectively. The flow-induced birefringence distribution was calculated with the linear stress-optical rule using the flow stresses, while the thermally-induced birefringence was calculated with the photoviscoelastic constitutive equation using the thermal stresses. They assumed that the flow- and thermally-induced residual stresses are not coupled and can be added to give the total residual stresses in the molded part. A similar assumption was made for the refractive index tensor. The numerical results of the flow-induced birefringence distribution show a peak away from the wall which is caused by the dominant effect of the first normal stress difference developed in the filling stage. The nonzero birefringence distribution in the core region is a consequence of the residual thermal birefringence. The numerical results were in agreement with measurements although some differences in location and magnitude of the peaks of birefringence were observed.
3.1 Governing Equations in Gas-Assisted Injection Molding

To describe the motion of any fluid the conservation equations of mass, momentum and energy are used. They detail how the mass, momentum, and energy are transported from one position of the medium to another during flow [68]. The conservation equations are nonlinear and coupled. This fact makes them difficult to solve. For some cases where the flow is isothermal, fully developed and the geometry is simple, e.g. in pipes and parallel plates, it is possible to obtain an analytical solution. For more complicated geometries, like Hele-Shaw cell and two- or three-dimensional problems, some terms of the conservation equations, that represent minor changes of density, velocity, stresses, and/or temperature, can be neglected. This simplification certainly introduces error and even with these considerations, in many cases, there is no an analytical solution. Therefore, numerical methods are implemented using the simplified equations in order to reduce the computational efforts [109]. In the numerical methods the flow domain is divided into non-overlapping subdomains called elements which are connected at specific points called nodes. The governing and constitutive equations, which form a set of differential equations, are discretized into an algebraic system of equations that are solved using numerical techniques. The solution of these equations at
the local elements is then related globally to the entire flow domain to reach an approximated solution.

The development of numerical techniques to predict the polymer melt flow in polymer processing operations is currently of paramount importance. In particular, viscoelastic computer simulations in GAIM will allow us to understand the polymer flow considering its viscoelastic nature during the gas penetration. To determine the residual stresses and final birefringence distribution in the moldings, calculations of pressure, shear and normal stresses, velocity and temperature profiles of the polymer melt through the mold region, including the position and shape of the advancing gas and melt fronts are required.

The numerical simulation of the whole non-isothermal GAIM process can be divided in its three basic stages: filling, primary gas penetration, and cooling. During the filling stage, the polymer melt enters the mold at constant temperature and constant volumetric flow rate. This results in the formation of the classical solid skin and the molten core structure observed in conventional injection molding. In the second stage the gas displaces the polymer melt in the core based on the time-dependent kinematics of interface evolution. The numerical solution of this process remains a challenging problem because the melt and gas front advancement is a transient moving-boundary flow problem [109]. The shape of the moving interface is unknown and must be determined as part of the solution of the governing equations for polymer melt and gas domains. To solve this kind of problems, a large number of iterations are usually required in order to track the shape of the moving boundary which evolves with time. In the cooling stage, due to the fact that the primary gas penetration is so rapid, it is considered that most of
the heat exchange between the molding and the mold takes place in this stage [31]. Therefore, essentially all of the density change occurs during this stage where the polymer flow has ceased and the secondary gas penetration takes place.

During the gas penetration stage, the gas and polymer melt domains are considered immiscible at the interface. Thus, the mechanism of gas penetration can be considered to be similar to the co-injection process [49, 110] where a fluid of much lower viscosity displaces another of higher viscosity in the mold cavity without mixing. Therefore, a set of conservation equations, mass, momentum, and energy, has to be solved for each domain in order to describe the GAIM process. The governing equations for the fluid motion are:

conservation of mass

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

(3-1)

conservation of momentum

\[
\frac{\partial}{\partial t}(\rho \mathbf{v}) = -[\nabla \cdot \rho \mathbf{v} \cdot \mathbf{v}] - \nabla p - (\nabla \cdot \tau) + \rho g
\]

(3-2)

For a non-isothermal process, the mass and momentum equations are coupled with the energy equation which is written as:

\[
\rho C_v \left(\frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T\right) = \kappa \nabla^2 T + \Phi
\]

(3-3)

where \(\rho\) is the fluid density; \(\mathbf{v}\) is the velocity vector; \(p\) is the pressure; \(\tau\) is the extra stress tensor; \(g\) is the gravity acceleration; \(C_v\) is the specific heat; \(\kappa\) is the thermal conductivity; \(T\) is the temperature, and \(\Phi\) is the viscous heating term.
The governing equations for gas and polymer domains are coupled with the
kinematic interface condition which relates the change in the free surface/moving
boundary position to the local fluid velocity. Because of the impermeable boundary
condition at the interface, the velocity of any fluid particle at the interface must be
tangential to it and when the boundary is moving, the normal velocity component of the
fluid particle must be equal to that of the interface. Therefore, the polymer/gas interface
deforms according to the instantaneous velocity field at the interface. The position of the
interface during the gas penetration determines the gas bubble thickness with time and, as
a consequence, the residual wall thickness can be resolved. In general, the time and space
dependent interface is written in its implicit form as:

\[ Z = \delta(x, y, t) \]  

(3-4)

where \( \delta \) is the polymer/gas interface position and is a function of a plane of reference \( x-y \)
and time.

The physical requirement that there is no mass flux through the interface and that
it has to move with the material surface, gives a kinematic boundary condition which has
to be fulfilled at the interface at all times. It can be expressed as:

\[ (\mathbf{v} - \mathbf{v}_\delta) \cdot \mathbf{n} = 0 \quad \text{or} \quad \frac{dm}{dt} = 0 \]  

(3-5)

where \( \mathbf{v} \) and \( \mathbf{v}_\delta \) are the velocity of the fluid and the velocity of the interface,
respectively, \( \mathbf{n} \) is the unit vector normal to the boundary and the derivative of \( m \) with
respect time indicates that there is no mass flux at the interface.

The kinematic boundary condition describes the local change of the free surface
elevation [49, 110] which, in its general form, can be written as:
\[
\frac{\partial \delta}{\partial t} + u \frac{\partial \delta}{\partial x} + v \frac{\partial \delta}{\partial y} = w
\]  

(3-6)

where \(\delta\) is the position of the interface; \(u\) and \(v\) are the velocity components at the interface and \(w\) is the velocity normal to the interface.

To solve the whole set of governing equations to predict the polymer/gas interface evolution it is necessary to make another assumption based on both the polymer and gas viscosities. Typically the polymer/gas viscosity ratio is on the order of \(10^8\), thus, due to the high viscosity of the polymer, its Reynolds number is on the order of \(10^{-3}\) [39] indicating that the viscous forces govern its motion and the inertial forces can be neglected. On the contrary, because of the low viscosity of the gas, its Reynolds number is on the order of \(10^2\) indicating that the inertial forces can not be neglected and the equation of motion becomes nonlinear. To avoid this problem, the gas is replaced by a fictitious fluid with a viscosity on the order of \(10^{-3}\) of the viscosity of the polymer melt [39, 49]:

\[
\eta_{gas} \geq 10^{-3}\eta_{pol}
\]  

(3-7)

where \(\eta_{gas}\) and \(\eta_{pol}\) are the viscosities of the gas or fictitious fluid and polymer, respectively.

With the substitution of the gas viscosity with that of the fictitious fluid and keeping the density of the fictitious fluid equal to that of the gas, the Reynolds number is reduced to the order of \(10^{-3}\). Consequently, the inertial terms of the equation of motion for the gas domain can be neglected [39].

Hereafter, fictitious fluid and gas terms are used indistinctly and the variables corresponding to the gas domain will be labeled with the subscript “gas” while those for
the polymer domain will be labeled with the subscript “pol”. The properties of the fictitious fluid are the following:

1. The pressure drop through the bubble length is negligible.

2. Its density and all other physical properties are the same as that of the gas.

The governing equations are complemented with a set of boundary and initial conditions, which depend on the problem geometry and are specified later for a particular case.

To calculate the polymer melt shrinkage due to temperature and pressure during the cooling process, the P-V-T equation of state proposed by Tait [12] is used.

\[ \rho(T, p) = \rho_0(T) \left[ 1 - C \ln \left\{ 1 + \frac{p}{B(T)} \right\} \right]^{-1} \]  
\( (3-8) \)

with \( \rho_0(T) = \frac{\rho_0(T_g^0)}{1 + \alpha_0(T_g^0)(T - T_g^0)} \)  
\( (3-9) \)

\[ \alpha = \alpha_l \text{ if } T > T_t \]  
\( (3-10) \)

\[ \alpha = \alpha_s \text{ if } T < T_t \]  
\( (3-11) \)

\[ B(T) = b_{1l} \exp(b_{2l}T) \text{ if } T > T_t \]  
\( (3-12) \)

\[ B(T) = b_{1s} \exp(b_{2s}T) \text{ if } T < T_t \]  
\( (3-13) \)

\[ T_t = T_g^0 + b_3 p \]  
\( (3-14) \)

where \( b_{1l}, b_{2l}, b_{1s}, b_{2s}, b_3 \) (subscripts \( l \) and \( s \) refer to liquid and solid state, respectively) are constants and \( T_t \) is the transition temperature (either \( T_g \) or \( T_m \)) and \( \alpha_l \) and \( \alpha_s \) are the thermal expansion coefficients for liquid and glassy states, respectively.
3.2 Flow-Induced Stresses and Birefringence

As mentioned earlier in Section 2.5, flow- and thermally-induced residual stresses are originated from two different phenomena. To date, no constitutive equation can describe the rheological behavior of a polymer in both solid and melt states. Thus, it is assumed that the coupling effects between the flow- and thermally-induced residual stresses and birefringence can be neglected and, as a consequence, they can be calculated separately [11, 104, 111].

To calculate the flow-induced residual stresses, it is necessary to take into consideration the build up and relaxation of stresses in the polymer melt during the filling and primary gas penetration stages. Consequently, the Leonov viscoelastic constitutive equation [6, 82] is implemented. The Leonov model was chosen for the present formulation because of the following reasons: a) its predictive capability is reasonably good in different flow situations [69, 112], b) the parameters of the Leonov model can be found using viscosity data obtained by simple shear test [91], and c) the relatively simple form of the Leonov model makes it feasible to implement in simulations [113].

Additionally, two or three modes are usually enough to describe the nonlinear response of the stress tensor during the polymer flow [91]. The Leonov model has been used in numerical calculations of flow-induced residual stresses [2,81] and is written as follows:

\[ \sigma = -p \delta + 2\eta_0 \varepsilon + \sum \frac{\eta_\kappa}{\theta_\kappa} C^{\kappa} \]  
\[ \varepsilon = \frac{1}{2} (\nabla v + \nabla v^T) \]

where \( \varepsilon \) is the deformation-rate tensor defined as:

The Leonov model has been used in numerical calculations of flow-induced residual stresses [2,81] and is written as follows:
and $\eta_0$ is the zero-shear-rate viscosity defined as:

$$\eta_v = \frac{\sum \eta_i}{1 - s}$$  \hfill (3-17)

$\mathbf{v}$ is the velocity vector; $p$ is the pressure; $s$ is a rheological parameter lying between zero and one; $K$ represents the number of modes; $\eta_K$ and $\theta_K$ are the $K^{\text{th}}$ mode shear viscosity and relaxation time, respectively, superscript $T$ means transpose and $\mathbf{C}_e$ is the elastic strain tensor which represents the portion of total strain which will be recovered if all the stresses on the viscoelastic fluid are suddenly released.

One of the techniques to characterize the molecular orientation in polymers is through the determination of the birefringence [8]. The flow-induced birefringence is calculated using the stress-optical rule which, in its general form, can be written as:

$$n_i - n_j = C(\sigma_i - \sigma_j)$$ \hfill (3-18)

where $C$ is the stress-optical coefficient; $n_i$ are the principal refractive index and $\sigma_i$ are the principal stresses.

It is considered that the stress-optical rule is applicable to unsteady non-isothermal flow and relaxation [81] and the flow birefringence developed during the flow gets frozen-in when the polymer reaches the glass transition temperature ($T_g$) [14].

### 3.3 Formulation of GAIM for One-Dimensional Tubular Cavity

In the following sections, the governing equations for the GAIM process are presented for one-dimensional tubular flow. The formulation takes into account the viscoelasticity of the polymer melt during the filling, primary gas and secondary gas penetration stages.
3.3.1 Governing Equations and Boundary Conditions

To implement the numerical solution for flow in a tubular cavity, the cylindrical coordinate system \((z, r, \theta)\) is used, with the \(z\)-axis being the flow direction, \(r\)-axis being the radial direction and \(\theta\)-axis being the angular direction. The velocity vector components in cylindrical coordinates are \(V(u,v,w)\). In the numerical implementation, the GAIM process is divided in its three main stages. During the filling stage, the polymer melt enters the cavity under a fully developed Poiseuille flow at uniform melt temperature, \(T_m\). During the primary gas penetration, the governing equations for both polymer and the fictitious fluid are coupled with the kinematic condition at the boundary, and in the third stage, the cooling process and the secondary gas penetration take place.

In order to simplify the governing equations, the following assumptions are made:

1. The polymer melt is considered incompressible during the filling and primary gas penetration stages.
2. Gravitational and inertial effects are neglected in the force balance due to the large viscosity of the polymer melt.
3. No-slip condition of the polymer at the mold wall.
4. The pressure is assigned to be zero at the melt front.
5. Pressure gradient in the flow direction is independent of the radial position.
6. The fountain flow effect at the melt front is not taken into account.
7. The thermal convection in the radial direction is negligible.
8. Heat conduction in the flow direction is negligible compared to heat conduction in the radial direction.
9. Thermal conductivity and heat capacity are assumed to be constants.
10. The mold wall temperature is constant.

11. Polymer and gas are not miscible at the interface.

During the filling stage, the radial and angular velocity components are zero, so the resulting velocity field is \( u = v_z(z, r) \) and \( v = w = 0 \) (assumption #6). Thus, the conservation equations of mass and momentum for an incompressible, non-isothermal fluid, for one-dimensional tubular cavity are reduced to:

\[
\frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial z} = -\rho \frac{\partial u}{\partial z} \tag{3-19}
\]

\[
\frac{1}{r} \frac{\partial}{\partial r} \left( \eta_r \frac{\partial u}{\partial r} \right) - \frac{\partial p}{\partial z} = 0 \tag{3-20}
\]

For a non-isothermal problem the energy equation which is written as:

\[
\rho \epsilon_c \left( \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial z} \right) = \frac{1}{r} \frac{\partial}{\partial r} \left( \kappa_n r \frac{\partial T}{\partial r} \right) + \Phi \tag{3-21}
\]

The generation of heat through the action of viscous dissipation leads to significant temperature variations along the shear direction. Because the viscosity of the polymer is highly dependent on temperature, the relationship between the stresses and shear rate is considerably altered by the local increase in temperature from viscous heating. According to Sobhanie and Isayev [108] the energy dissipation function for a viscoelastic fluid, can be written as:

\[
\Phi = 2s \eta_0 tr(e^\circ) + \sum_{\epsilon} \frac{\eta_0}{4\theta_\epsilon} \left[ \frac{1}{3} tr(C_{\epsilon}^i) \cdot \left\{ tr(C_{\epsilon}^i) - tr(C_{\epsilon}^j) \right\} + tr(C_{\epsilon}^j) - 3 \right] \tag{3-22}
\]

where \( e \) is the deformation-rate tensor defined by Eq. (3-16) and \( \eta_0 \) is the zero-shear-rate viscosity defined by Eq. (3-17).
To solve the set of equations that govern the motion of the fluid, it is necessary to specify the initial and boundary conditions. The initial condition for the temperature of the melt is written as:

\[ T = T_m \quad \text{at} \quad t = 0 \tag{3-23} \]

where \( T_m \) is the polymer melt temperature and \( t \) stands for time.

The boundary conditions for the velocity component in the flow direction \((u)\), temperature, pressure, and flow rate for tubular flow in cylindrical coordinates are:

\[ u|_{r=\pm R} = 0 \tag{3-24} \]

\[ \frac{\partial u}{\partial r}|_{r=0} = 0 \tag{3-25} \]

\[ T|_{r=\pm R} = T_w \tag{3-26} \]

\[ \frac{\partial T}{\partial r}|_{r=0} = 0 \tag{3-27} \]

\[ \frac{\partial p}{\partial r} = 0 \quad \text{no penetration at the all solid boundaries} \tag{3-28} \]

\[ Q = Q_{\text{ent}} \quad \text{or} \quad p = p_{\text{ent}} \tag{3-29} \]

where \( T_w \) is the mold temperature, \( R \) is the radius of the tube which can vary along the flow direction, \( Q_{\text{ent}} \) and \( p_{\text{ent}} \) are the flow rate and pressure at the entrance node, respectively.

### 3.3.2 Pressure Development in Filling Stage

In the filling stage, the polymer melt is considered incompressible [114]. Hence, the equation of motion (Eq. (3-20)) in terms of stresses reduces to:
\[ \frac{1}{r} \frac{\partial}{\partial r} (r \tau_{r_z}) = \frac{\partial p}{\partial z} \]  

(3-30)

For the polymer melt domain, it is considered that the pressure gradient in the flow direction is independent of the radius (assumption 5). Thus, the equation of motion can be integrated with respect to \( r \) and using the boundary condition in Eq. (3-25) it gives:

\[ \tau_{r_z} = \frac{\partial p}{\partial z} \frac{r}{2} \]  

(3-31)

Expanding the Leonov equation (Eq. (3-15)) for a one dimensional tubular flow we have:

\[
\begin{vmatrix}
\sigma_{rr} & 0 & \tau_{r_z} \\
0 & \sigma_{zz} & 0 \\
\tau_{r_z} & 0 & \sigma_{zz}
\end{vmatrix} = 
\begin{vmatrix}
-p & 0 & 0 \\
0 & -p & 0 \\
0 & 0 & -p
\end{vmatrix} + \eta_s \begin{vmatrix}
0 & 0 & \frac{\partial u}{\partial r} \\
0 & 0 & 0 \\
\frac{\partial u}{\partial r} & 0 & 0
\end{vmatrix} + \sum_{k=1}^{\infty} \frac{\eta_k}{\theta_k} \begin{vmatrix}
C_{\sigma,\sigma} & 0 & C_{\sigma,\tau} \\
0 & C_{\sigma,\sigma} & 0 \\
C_{\tau,\sigma} & 0 & C_{\tau,\tau}
\end{vmatrix}
\]

(3-32)

Because of the symmetry in shear stresses \( \tau_{r_z} = \tau_{zr} \) the resulting stress components for one-dimensional tubular flow are:

\[ \sigma_{rr} = -p + \sum_{k=1}^{\infty} \frac{\eta_k}{\theta_k} C_{\sigma,\sigma} \]  

(3-33)

\[ \sigma_{zz} = -p + \sum_{k=1}^{\infty} \frac{\eta_k}{\theta_k} C_{\sigma,\sigma} \]  

(3-34)

\[ \sigma_{zz} = -p + \sum_{k=1}^{\infty} \frac{\eta_k}{\theta_k} C_{\sigma,\sigma} \]  

(3-35)

\[ \tau_{r_z} = \eta_s \frac{\partial u}{\partial r} + \sum_{k=1}^{\infty} \frac{\eta_k}{\theta_k} C_{\tau,\tau} \]  

(3-36)
Substituting the shear stress component (Eq. (3-36)) into the momentum equation (Eq. (3-31)) we obtain:

\[
\frac{\partial p}{\partial z} \frac{r}{2} = \eta_s \frac{\partial u}{\partial r} + \sum_{k=1}^{N^2} \eta_k \frac{C_{r,k}}{\theta_k} \tag{3-37}
\]

Eq. (3-37) can be rewritten as:

\[
\frac{\partial p}{\partial z} \frac{r}{2} = \left[ \eta_s \frac{\partial u}{\partial r} + \sum_{k=1}^{N^2} \eta_k \frac{C_{r,k}}{\theta_k} \right] \frac{\partial u}{\partial r} \tag{3-38}
\]

Simplifying Eq. (3-38) and solving for the shear rate, we obtain:

\[
\frac{\partial u}{\partial r} = \frac{\partial p}{\partial z} \frac{r}{2\eta_z} \tag{3-39}
\]

where \(\eta_z\) is the pseudo viscosity function [108] defined as:

\[
\eta_z = \eta_s + \sum_{k=1}^{N^2} \eta_k \frac{C_{r,k}}{\theta_k} \frac{\partial u}{\partial r} \tag{3-40}
\]

Integrating Eq. (3-39) with respect to the radius, we obtain:

\[
u(R) - u(r) = \frac{\partial p}{\partial z} \frac{1}{2} \int_r^R \frac{r'}{\eta_z} dr' \tag{3-41}
\]

Considering the no-slip condition (Eq. (3-24)) Eq. (3-41) reduces to:

\[
u(r) = -\frac{\partial p}{\partial z} \frac{1}{2} \int_0^r \frac{r}{\eta_z} dr' \tag{3-42}
\]

Multiplying Eq. (3-42) by \(2r/R^3\) and integration over the whole radius of the cavity, we obtain:
\[
\frac{2}{R} \int_{\overline{R}}^{\overline{R}} u(\overline{r}) \overline{r} d\overline{r} = - \frac{1}{R^2} \frac{\partial p}{\partial z} \int_{\overline{R}}^{\overline{R}} \left( \frac{r^2}{\eta_t} \right) r d\overline{r} 
\]

(3-43)

The left hand side of Eq. (3-43) represents the average velocity, \( \overline{u} \), for one-dimensional flow and is defined as [84]:

\[
\overline{u} = \frac{2}{R} \int_{\overline{R}}^{\overline{R}} u(r) \overline{r} d\overline{r} 
\]

(3-44)

Integrating the continuity equation (Eq. (3-19)) for an incompressible one-dimensional tubular Poiseuille flow, the mass conservation equation in terms of the average velocity is written as [84]:

\[
\frac{\partial R^2 \overline{u}}{\partial z} = 0 
\]

(3-45)

Combining Eqs. (3-43) and (3-44), solving for the average velocity and substituting it into Eq. (3-45) we obtain:

\[
\frac{\partial}{\partial z} \left( \frac{\partial p}{\partial z} \int_{\overline{R}}^{\overline{R}} \left( \frac{r^2}{\eta_t} \right) r d\overline{r} \right) = 0 
\]

(3-46)

Eq. (3-46) can be rewritten as:

\[
\frac{\partial}{\partial z} \left( S \frac{\partial p}{\partial z} \right) = 0 
\]

(3-47)

with

\[
S = \int_{\overline{R}}^{\overline{R}} \left( \frac{r^2}{\eta_t} \right) r d\overline{r} 
\]

(3-48)

Eq. (3-47) is the primary governing equation of one-dimensional tubular flow in the filling stage during GAIM process.
3.3.3 Gas Penetration Dynamics

During the gas penetration stage, a complete set of governing equations have to be solved for each domain. With the introduction of the fictitious fluid concept, the conservation equations of mass and momentum (Eqs. (3-1) and (3-2)) for both gas and polymer in one-dimensional circular tube reduce to [115]:

\[
\frac{\partial \rho_i}{\partial t} + \frac{\partial \rho_i u_i}{\partial z} + \frac{1}{r} \frac{\partial}{\partial r} \left( \rho_i w_i \right) = 0
\] (3-49)

\[
\frac{1}{r} \frac{\partial}{\partial r} \left( r \tau_{rz,i} \right) - \frac{\partial p}{\partial z} = 0
\] (3-50)

where \( i = \text{“gas” or “pol”} \) and represents the gas or polymer domain, respectively, \( z \) and \( r \) represent the flow and radial directions, respectively, \( p \) is the pressure, \( u \) and \( w \) are the velocities in the \( z \) and \( r \) directions, respectively, and \( \rho_i \) is the density.

The governing equations are coupled by the kinematic boundary condition which for a one-dimensional flow in cylindrical coordinates Eq. (3-6) is reduced to:

\[
w_i^g = \frac{\partial \delta}{\partial t} + u_i^g \frac{\partial \delta}{\partial z}
\] (3-51)

where \( i = \text{“gas” or “pol”} \) and represents the gas and polymer domain, respectively, and \( \delta \) represents the polymer/gas interface position in the radial direction (half diameter of the gas domain).

Eq. (3-51) is coupled with both mass and momentum conservation equations for melt and gas, and its solution indicates the interface location.
3.3.4 Mass Continuity Equation for Gas Domain

The mass continuity equation for the fictitious fluid (Eq. 3-49), which is considered compressible during the molding process, is integrated over the radius in the gas domain giving the following expression:

\[ \int_0^s r \frac{\partial \rho_{\text{gas}}}{\partial t} dr + \int_0^s r \frac{\partial \left( \rho_{\text{gas}} u_{\text{gas}} \right)}{\partial z} dr + \int_0^s \frac{\partial \left( \rho_{\text{gas}} w_{\text{gas}} \right)}{\partial r} dr = 0 \]  

(3-52)

The radial velocity of the gas is considered zero at the center line, \( w_{\text{gas}} = 0 \) at \( r = 0 \). Thus Eq. (3-52) reduces to:

\[ \int_0^s r \frac{\partial \rho_{\text{gas}}}{\partial t} dr + \int_0^s r \frac{\partial \left( \rho_{\text{gas}} u_{\text{gas}} \right)}{\partial z} dr + \rho_{\text{gas}} \left| \delta w_{\text{gas}} \right| = 0 \]  

(3-53)

Substituting the kinematic interface condition Eq. (3-51) in the third term of Eq. (3-53) we have:

\[ \int_0^s r \frac{\partial \rho_{\text{gas}}}{\partial t} dr + \int_0^s r \frac{\partial \left( \rho_{\text{gas}} u_{\text{gas}} \right)}{\partial z} dr + \rho_{\text{gas}} \left| \delta w_{\text{gas}} \right| \delta \left( \frac{\partial \delta}{\partial t} + u_{\text{gas}} \frac{\partial \delta}{\partial z} \right) = 0 \]  

(3-54)

Applying the Leibniz integral rule on the second term of Eq. (3-54) leads to:

\[ \int_0^s r \frac{\partial \rho_{\text{gas}}}{\partial t} dr + \frac{\partial}{\partial z} \int_0^s \rho_{\text{gas}} u_{\text{gas}} dr - \rho_{\text{gas}} \left| \delta u_{\text{gas}} \right| \frac{\partial \delta}{\partial z} + \rho_{\text{gas}} \left| \delta u_{\text{gas}} \right| \delta \left( \frac{\partial \delta}{\partial t} + u_{\text{gas}} \frac{\partial \delta}{\partial z} \right) = 0 \]  

(3-55)

Simplifying Eq. (3-55), we obtain the mass continuity equation for gas domain:

\[ \int_0^s r \frac{\partial \rho_{\text{gas}}}{\partial t} dr + \frac{\partial}{\partial z} \int_0^s \rho_{\text{gas}} u_{\text{gas}} dr + \rho_{\text{gas}} \left| \delta u_{\text{gas}} \right| \frac{\partial \delta}{\partial t} = 0 \]  

(3-56)

3.3.5 Mass Continuity Equation for Polymer Domain

Similarly, integration of the mass continuity equation (Eq. (3-49)) on the polymer domain along the radius leads to:
\[
\int_{\delta}^{R} \frac{\partial \rho_{\text{pol}}}{\partial t} dr + \int_{\delta}^{R} r \frac{\partial (\rho_{\text{pol}} u_{\text{pol}})}{\partial z} dr + \int_{\delta}^{R} \frac{\partial (\rho_{\text{pol}} r w_{\text{pol}})}{\partial r} dr = 0
\]  

(3-57)

Integrating the third term in the left hand side of Eq. (3-57), considering that the mold boundaries are impermeable, and the velocity component \(w_{\text{pol}} = 0\) at \(r = R\), Eq. (3-57) reduces to:

\[
\int_{\delta}^{R} \frac{\partial \rho_{\text{pol}}}{\partial t} dr + \int_{\delta}^{R} r \frac{\partial (\rho_{\text{pol}} u_{\text{pol}})}{\partial z} dr - \rho_{\text{pol}} \frac{\delta}{\delta_{\text{pol}}} \delta w_{\text{pol}} = 0
\]  

(3-58)

Substituting the kinematic interface condition (Eq. (3-51)) into Eq. (3-58) one obtain:

\[
\int_{\delta}^{R} \frac{\partial \rho_{\text{pol}}}{\partial t} dr + \int_{\delta}^{R} r \frac{\partial (\rho_{\text{pol}} u_{\text{pol}})}{\partial z} dr - \rho_{\text{pol}} \frac{\delta}{\delta_{\text{pol}}} \delta \left( \frac{\partial \delta}{\partial t} + u_{\text{pol}} \frac{\partial \delta}{\partial z} \right) = 0
\]  

(3-59)

Applying the Leibniz integral rule to the second term on the left hand side of Eq. (3-59) we have:

\[
\int_{\delta}^{R} \frac{\partial \rho_{\text{pol}}}{\partial t} dr + \frac{\partial}{\partial z} \left[ \int_{\delta}^{R} \rho_{\text{pol}} r u_{\text{pol}} dr + \rho_{\text{pol}} \left|_{\delta} \right. \frac{\partial \delta}{\partial z} \frac{\partial \delta}{\partial \text{pol}} \delta u_{\text{pol}} \left|_{\delta} \right. - \rho_{\text{pol}} \left|_{\delta} \right. \frac{\partial \delta}{\partial t} + u_{\text{pol}} \left|_{\delta} \right. \frac{\partial \delta}{\partial z} \right] = 0
\]  

(3-60)

Simplifying Eq. (3-60) we obtain the mass continuity equation for the polymer domain:

\[
\int_{\delta}^{R} \frac{\partial \rho_{\text{pol}}}{\partial t} dr + \frac{\partial}{\partial z} \left[ \int_{\delta}^{R} \rho_{\text{pol}} r u_{\text{pol}} dr - \rho_{\text{pol}} \left|_{\delta} \right. \frac{\partial \delta}{\partial t} \right] = 0
\]  

(3-61)

3.3.6 Equation of Motion for Gas Domain

Integrating the equation of motion (Eq. (3-50)) with respect the radius over the gas domain we get:

\[
\tau_{\text{rc, gas}} = \frac{r}{2} \frac{\partial p}{\partial z} + C_1 \quad 0 \leq r \leq \delta
\]  

(3-62)
According to the boundary condition in Eq. (3-25) the shear stress at the center line is zero \( \tau_{rz, \text{gas}}\big|_{r=0} = 0 \). Therefore, the integration constant, \( C_i \), vanishes and Eq. (3-62) reduces to:

\[
\tau_{rz, \text{gas}} = \frac{r \partial p}{2 \partial z} \quad 0 \leq r \leq \delta
\]  

(3-63)

Evaluation of shear stresses in Eq. (3-63) at the interface \( r = \delta \) results in:

\[
\tau_{rz, \text{gas}}\big|_{\delta} = \frac{\delta \partial p}{2 \partial z}
\]  

(3-64)

Considering that the fictitious fluid that represents the gas domain behaves like a Newtonian fluid, Eq. (3-63) can be rewritten in terms of the velocity components as:

\[
\frac{\partial u_{gas}}{\partial r} = \frac{r \partial p}{2 \eta_{gas} \partial z} \quad 0 \leq r \leq \delta
\]  

(3-65)

Integration of Eq. (3-65) with respect to radius we obtain the equation of motion for the gas domain, written as follows:

\[
u_{gas} \big|_\delta - u_{gas} \big|_r = \frac{1}{\eta_{gas}} \int_{r}^{\delta} \frac{r \partial p}{\partial z} dr \quad 0 \leq r \leq \delta
\]  

(3-66)

3.3.7 Equation of Motion for Polymer Domain

Integrating the equation of motion with respect the radius over the polymer domain we have:

\[
\tau_{rz, \text{pol}} = \frac{r \partial p}{2 \partial z} + C_2 \quad \delta \leq r \leq R
\]  

(3-67)

To find the integration constant \( C_2 \) we make use of the boundary condition at the interface. It has been demonstrated by Palluch and Isayev [116] that the presence of
viscoelastic normal stresses at the interface in transient multiphase flow, creates a discontinuity in shear stress at the interface between the two fluids. As a first approximation, in this case, it is considered that the shear stress is continuous throughout both polymer and gas domains. Then, the shear stress for both domains at the polymer/gas interface is identical:

$$\tau_{\text{rz, gas}}|_{\delta} = \tau_{\text{rz, pol}}|_{\delta}$$  

(3-68)

Evaluation of Eq (3-67) at the interface $r=\delta$ results in:

$$\tau_{\text{rz, pol}}|_{\delta} = \frac{\delta}{2} \frac{\partial p}{\partial z} + C_2$$  

(3-69)

Substituting Eq. (3-64) into Eq. (3-68) and further substitution into Eq. (3-69) the integration constant, $C_2$, vanishes. Then, combining Eqs. (3-67) and (3-69) we obtain the following equation for shear stresses in the polymer domain:

$$\tau_{\text{rz, pol}} - \tau_{\text{rz, pol}}|_{\delta} = \frac{1}{2} \frac{\partial p}{\partial z} (r - \delta) \quad \delta \leq r \leq R$$  

(3-70)

To consider the viscoelasticity of the polymer, the shear stresses are expressed by the Leonov equation. Thus, from Eq. (3-36) we get:

$$\tau_{\text{rz, pol}} = \eta_s \frac{\partial u_{\text{pol}}}{\partial r} + \sum_{k=1}^{N} \eta_k \frac{\partial u_{\text{pol}}}{\partial r} C_{\text{r, k}}$$  

(3-71)

Eq. (3-71) can be rewritten as:

$$\tau_{\text{rz, pol}} = \left[ \sum_{k=1}^{N} \frac{\eta_k}{\theta_k} C_{\text{r, k}} \right] \frac{\partial u_{\text{pol}}}{\partial r}$$  

(3-72)

Simplifying Eq. (3-72) we obtain:
\[ \tau_{rz,\text{pol}} = \eta_z \frac{\partial u_{pol}}{\partial r} \]  

(3-73)

where \( \eta_z \) is the pseudo viscosity which has been defined previously in Eq. (3-40).

Substituting Eq. (3-73) into Eq. (3-70) we obtain the equation of motion for the polymer domain:

\[ \eta_z \frac{\partial u_{pol}}{\partial r} - \tau_{rz,\text{pol}} \bigg|_{\delta} = \frac{1}{2} \frac{\partial p}{\partial z} (r - \delta) \quad \delta \leq r \leq R \]  

(3-74)

3.3.8 Transient Evolution Equation for Polymer and Gas Domains

As stated before, a sharp interface is assumed to exist between the gas and polymer domains. But, the dynamic boundary condition requires that the stresses acting on the fluids at the moving interface to be in equilibrium and continuous. Thus, using the equality in Eq. (3-68) and combining Eqs. (3-64) and (3-74) we obtain:

\[ \frac{\partial u_{pol}}{\partial r} = \frac{r}{2 \eta_z} \frac{\partial p}{\partial z} \quad \delta \leq r \leq R \]  

(3-75)

Integrating Eq. (3-75) over the polymer domain we obtain:

\[ u_{pol} \bigg|_\delta - u_{pol} \bigg|_0 = \frac{1}{2} \frac{\partial p}{\partial z} \int_\delta^R \frac{r}{\eta_z} dr \quad \delta \leq r \leq R \]  

(3-76)

Using the no slip boundary condition (Eq.(3-24)) \( u_{pol} \bigg|_{r=R} = 0 \), Eq. (3-76) reduces to:

\[ u_{pol} \bigg|_\delta = \frac{-1}{2} \frac{\partial p}{\partial z} \int_\delta^R \frac{r}{\eta_z} dr \quad \delta \leq r \leq R \]  

(3-77)

Since the velocity of both the fictitious fluid and the polymer at the interface are considered to be equal \( u_{gas} \bigg|_\delta = u_{pol} \bigg|_0 \), combining Eqs. (3-66) and (3-77) results in:
This equation describes the velocity of the gas domain in the flow direction.

Multiplication of Eq. (3-78) by $\rho_{\text{gas}} r$ and integration over the gas domain leads to the following expression:

$$
\int_{\delta}^{\delta} \rho_{\text{gas}} u_{\text{gas}} dr = -\frac{1}{2} \frac{\partial p}{\partial z} \left[ \int_{\delta}^{\delta} \frac{r \cdot \rho_{\text{gas}}}{\eta_{\text{gas}}} dr + \int_{\delta}^{\delta} \frac{r \cdot \rho_{\text{gas}}}{\eta_z} dr \right]
$$

(3-79)

Simplifying the previous equation results in:

$$
\int_{\delta}^{\delta} \rho_{\text{gas}} u_{\text{gas}} dr = -\frac{1}{2} \frac{\partial p}{\partial z} \left[ \int_{\delta}^{\delta} \frac{r \cdot \rho_{\text{gas}}}{\eta_{\text{gas}}} \left( \int_{0}^{\delta} r \cdot \rho_{\text{gas}} dr + \int_{\delta}^{\delta} \frac{r \cdot \rho_{\text{gas}}}{\eta_z} dr \right) \right]
$$

(3-80)

$$
\int_{\delta}^{\delta} \rho_{\text{gas}} u_{\text{gas}} dr = -\frac{1}{2} \frac{\partial p}{\partial z} S_{\text{gas}}
$$

(3-81)

with

$$
S_{\text{gas}} = \left( \int_{\delta}^{\delta} \frac{r \cdot \rho_{\text{gas}}}{\eta_{\text{gas}}} \left( \int_{0}^{\delta} \rho_{\text{gas}} \cdot r dr + \int_{\delta}^{\delta} \frac{\rho_{\text{gas}} \cdot r dr}{\eta_z} \right) \right)
$$

(3-82)

Substituting Eq. (3-81) into the mass continuity equation for gas domain (Eq. (3-56)) and multiplying by $\frac{2}{\rho_{\text{gas}}}$ gives the gas domain interface evolution equation:

$$
\frac{2}{\rho_{\text{gas}}} \int_{\delta}^{\delta} \frac{\partial \rho_{\text{gas}}}{\partial t} dr + \frac{\partial \delta^2}{\partial t} + \frac{\partial}{\partial z} \left( -\frac{\partial p}{\partial z} S_{\text{gas}} \right) = 0
$$

(3-83)

with

$$
S_{\text{gas}} = \left( \int_{\delta}^{\delta} \frac{r \cdot \rho_{\text{gas}}}{\eta_{\text{gas}}} \left( \int_{0}^{\delta} \rho_{\text{gas}} \cdot r dr + \int_{\delta}^{\delta} \frac{\rho_{\text{gas}} \cdot r dr}{\eta_z} \right) \right)
$$

(3-84)

Combining Eqs. (3-76) and (3-77) results in:
\[ u_{pol} = \frac{1}{2} \frac{\partial p}{\partial z} \int_{\delta}^{r} \frac{r}{\eta_z} dr - \frac{1}{2} \frac{\partial p}{\partial z} \int_{\delta}^{r} \frac{r}{\eta_z} dr \]  

(3-85)

Combining both terms of the right hand side of Eq. (3-85) under one integral sign we have:

\[ u_{pol} = -\frac{1}{2} \frac{\partial p}{\partial z} \int_{\delta}^{r} \frac{r}{\eta_z} dr \]  

(3-86)

Multiplying Eq. (3-86) by \( \rho_{pol} r' \) and integrating over the polymer domain leads to:

\[ \int_{\delta}^{R} \rho_{pol} r' u_{pol} dr' = -\frac{1}{2} \frac{\partial p}{\partial z} \int_{\delta}^{r} \rho_{pol} r' \int_{\delta}^{r} \frac{r}{\eta_z} dr dr' \]  

(3-87)

Simplifying Eq. (3-87) we have:

\[ \int_{\delta}^{R} \rho_{pol} r' u_{pol} dr' = -\frac{1}{2} \frac{\partial p}{\partial z} \int_{\delta}^{r} \rho_{pol} r' dr' \]  

(3-88)

\[ \int_{\delta}^{R} \rho_{pol} r' u_{pol} dr' = -\frac{1}{2} \frac{\partial p}{\partial z} S_{pol} \]  

(3-89)

with

\[ S_{pol} = \int_{\delta}^{R} \int_{\delta}^{r} \rho_{pol} r' dr' \]  

(3-90)

Substituting Eq. (3-89) into the mass continuity equation for polymer domain (Eq. (3-61)) and multiplying by \( \frac{2}{\rho_{pol} |_{\delta}} \) gives the polymer domain interface evolution equation.

\[ \frac{2}{\rho_{pol} |_{\delta}} \int_{\delta}^{R} r \frac{\partial \rho_{pol}}{\partial t} dr - \frac{\partial \delta^2}{\partial t} + \frac{\partial}{\partial z} \left( -\frac{\partial p}{\partial z} S_{pol} \right) = 0 \]  

(3-91)

with
\[ S_{\text{pol}} = \int_{\delta}^{r} \int_{\delta}^{r} \frac{\rho_{\text{pol}}}{\rho_{\text{pol}}} r'dr'dr \] (3-92)

Because of the dependence of the density on temperature and pressure which in turn depends on time, one can apply the calculus chain rule on the first term of the left-hand side of Eq. (3-83) which results in:

\[ \frac{2}{\rho_{\text{gas}}} \int_{0}^{\delta} r \frac{\partial \rho_{\text{gas}}}{\partial t} dr = \frac{2}{\rho_{\text{gas}}} \int_{0}^{\delta} r \left( \frac{\partial \rho_{\text{gas}}}{\partial p} \frac{\partial p}{\partial t} + \frac{\partial \rho_{\text{gas}}}{\partial T} \frac{\partial T}{\partial t} \right) dr \] (3-93)

Then, Eq. (3-93) can be rewritten as:

\[ \frac{2}{\rho_{\text{gas}}} \int_{0}^{\delta} r \frac{\partial \rho_{\text{gas}}}{\partial t} dr = G_{\text{gas}} \frac{\partial p}{\partial t} + H_{\text{gas}} \] (3-94)

with

\[ G_{\text{gas}} = \frac{2}{\rho_{\text{gas}}} \int_{0}^{\delta} r \left( \frac{\partial \rho_{\text{gas}}}{\partial p} \right) \frac{\partial p}{\partial t} dr \] (3-95)

and

\[ H_{\text{gas}} = \frac{2}{\rho_{\text{gas}}} \int_{0}^{\delta} r \left( \frac{\partial \rho_{\text{gas}}}{\partial T} \right) \frac{\partial T}{\partial t} dr \] (3-96)

Similarly for the polymer domain, one can apply the chain rule on the first term of the left-hand side of Eq. (3-91) which results in:

\[ \frac{2}{\rho_{\text{pol}}} \int_{\delta}^{R} r \frac{\partial \rho_{\text{pol}}}{\partial t} dr = \frac{2}{\rho_{\text{pol}}} \int_{\delta}^{R} r \left( \frac{\partial \rho_{\text{pol}}}{\partial p} \frac{\partial p}{\partial t} + \frac{\partial \rho_{\text{pol}}}{\partial T} \frac{\partial T}{\partial t} \right) dr \] (3-97)

Eq. (3-97) can be rewritten as:

\[ \frac{2}{\rho_{\text{pol}}} \int_{\delta}^{R} r \frac{\partial \rho_{\text{pol}}}{\partial t} dr = G_{\text{pol}} \frac{\partial p}{\partial t} + H_{\text{pol}} \] (3-98)

with
\[ G_{pol} = \frac{2}{\rho_{pol}} \int_{\delta}^{R} r \left( \frac{\partial \rho_{pol}}{\partial p} \right) \frac{\partial T}{\partial p} \, dr \] (3-99)

and

\[ H_{pol} = \frac{2}{\rho_{pol}} \int_{\delta}^{R} r \left( \frac{\partial \rho_{pol}}{\partial T} \right) \frac{\partial \rho_{pol}}{\partial T} \, dr \] (3-100)

Substituting Eqs. (3-94) and (3-98) into Eqs. (3-83) and (3-91), respectively, we obtain:

\[ G_{gas} \frac{\partial p}{\partial t} + H_{gas} + \frac{\partial \delta^2}{\partial t} + \frac{\partial}{\partial z} \left( -\delta \frac{\partial S_{gas}}{\partial z} \right) = 0 \] (3-101)

\[ G_{pol} \frac{\partial p}{\partial t} + H_{pol} - \frac{\partial \delta^2}{\partial t} + \frac{\partial}{\partial z} \left( -\frac{\partial p}{\partial z} S_{pol} \right) = 0 \] (3-102)

Eqs. (3-101) and (3-102) are the transient interface evolution equations for tracking the polymer/gas interface evolution. Solving for \( \frac{\partial \delta^2}{\partial t} \) and combining these two equations gives the following governing equations for both melt and gas flow in the whole cavity domain which can be used to solve the pressure gradient distribution and velocity field:

\[ G \frac{\partial p}{\partial t} + H + \frac{\partial}{\partial z} \left( -\frac{\partial p}{\partial z} S \right) = 0 \] (3-103)

with

\[ S = S_{gas} + S_{pol} \] (3-104)

where \( S_{gas} \) and \( S_{pol} \) were defined previously in Eqs. (3-84) and (3-92), respectively.

\[ G = G_{gas} + G_{pol} \] (3-105)

where \( G_{gas} \) and \( G_{pol} \) were defined previously in Eqs. (3-95) and (3-99), respectively.
and

\[ H = H_{gas} + H_{pol} \]  \hspace{1cm} (3-106)

where \( H_{gas} \) and \( H_{pol} \) were defined previously in Eqs. (3-96) and (3-100), respectively.

3.4 Primary Gas Penetration

Because the pressure losses in the gas domain are negligible, the pressure of the fictitious fluid that represents the gas is considered constant during the primary gas penetration. Also, due to the low thermal conductivity of the gas, the temperature variation in the gas domain is assumed small and its density is considered constant. Hence, both terms \( G_{gas} \) and \( H_{gas} \) in Eqs. (3-105) and (3-106), are neglected. Then, during the primary gas penetration, the compressibility of the polymer melt and the fictitious fluid is assumed to be negligible. Therefore, the governing equation for both melt and gas flow in the whole cavity (Eq. (3-103)), which is used to solve for the pressure gradient and velocity field distributions for one-dimensional tubular flow in the primary gas penetration stage, is written as:

\[ \frac{\partial}{\partial z} \left( \frac{\partial p}{\partial z} S \right) = 0 \]  \hspace{1cm} (3-107)

with

\[ S = \int_0^\delta \frac{r^3}{2\eta_{gas}} dr + \int_\delta^z \frac{r^3}{2\eta_z} dr \]  \hspace{1cm} (3-108)

The interface evolution equation for the gas domain yields:

\[ \frac{\partial \delta^2}{\partial t} + \frac{\partial}{\partial z} \left( -S_{gas} \frac{\partial p}{\partial z} \right) = 0 \]  \hspace{1cm} (3-109)
with

\[ S_{\text{gas}} = \int_{\delta}^{\eta_2} \frac{r'}{2\eta_{\text{gas}}} dr + \delta \int_{\eta_2}^{\eta_3} \frac{r'}{2\eta_z} dr \]  \hspace{1cm} (3-110)

And the interface evolution equation for polymer domain results in:

\[ \frac{\partial (R^2 - \delta^2)}{\partial t} + \frac{\partial}{\partial z} \left( - S_{\text{pol}} \frac{\partial p}{\partial z} \right) = 0 \]  \hspace{1cm} (3-111)

with

\[ S_{\text{pol}} = \int_{\delta}^{\eta_2} \frac{r (r^2 - \delta^2)}{2\eta_z} dr \]  \hspace{1cm} (3-112)

3.5 Secondary Gas Penetration

Polymer density variation due to the gas pressure and temperature during the cooling process causes the secondary gas penetration. To calculate the secondary gas penetration, the terms of the governing equation that represent the density variation of the polymer with respect to pressure \( G_{\text{pol}} \) and temperature \( H_{\text{pol}} \) defined in Eqs. (3-99) and (3-100), respectively, are taken into account. Thus, equation (3-103) yields to:

\[ G_{\text{pol}} \frac{\partial p}{\partial t} + H_{\text{pol}} + \frac{\partial}{\partial z} \left( - \frac{\partial p}{\partial z} S \right) = 0 \]  \hspace{1cm} (3-113)

with

\[ S = \int_{\delta}^{\eta_2} \frac{r^3}{2\eta_{\text{gas}}} dr + \delta \int_{\eta_2}^{\eta_3} \frac{r^3}{\eta_z} dr + \int_{\eta_2}^{\eta_3} \frac{\rho_{\text{pol}}}{\eta_z} \rho_{\text{pol}}' r dr dr \]  \hspace{1cm} (3-114)

Considering that the gas pressure is constant with respect to time in the gas domain and its density change is negligible, the interface evolution equation (Eq. (3-101) reduces to:
\[
\frac{\partial \delta^2}{\partial t} + \frac{\partial}{\partial z} \left( -S_{gas} \frac{\partial p}{\partial z} \right) = 0
\]  
(3-115)

with

\[
S_{gas} = \int_0^\delta \frac{r^3}{2\eta_{gas}} dr + \delta^2 \int_0^\delta \frac{r}{\eta_z} dr
\]  
(3-116)

The interface evolution equation for the polymer domain remains the same as Eq. (3-102).

3.6 Elastic Strain Tensor of Leonov Model

The flow stress field (\(\sigma\)) developed during the filling and gas penetration stages, is calculated using the Leonov model for incompressible fluids (Eq. (3-15)). The elastic strain tensor \(C_{\varepsilon, k}\) of Eq. (3-15) is governed by the following evolution equation [82]:

\[
2\theta\varepsilon \frac{\partial}{\partial t} C_{\varepsilon, k} + \left[ C_{\varepsilon, k} + C_{\varepsilon, k} \left( \frac{II - I}{3} \right) - \delta \right] = 0
\]  
(3-117)

where I and II are the first and second invariants of the elastic strain tensor \(C_{\varepsilon, k}\), respectively, and \(\frac{\partial}{\partial t} C_{\varepsilon, k}\) is the upper convected Jaumann derivative of the elastic strain tensor defined as [73]:

\[
\frac{\partial}{\partial t} C_{\varepsilon, k} = \frac{D}{Dt} C_{\varepsilon, k} - \nabla \cdot \nabla C_{\varepsilon, k} - C_{\varepsilon, k} \cdot \nabla \nabla
\]  
(3-118)

where D/Dt is the differential operator of the substantial derivative of the elastic strain tensor defined as:

\[
\frac{D}{Dt} C_{\varepsilon, k} = \frac{\partial}{\partial t} C_{\varepsilon, k} + \nabla \cdot \nabla C_{\varepsilon, k}
\]  
(3-119)
Expanding Eq. (3-117), the evolution equation for the elastic strain tensor of the
Leonov model \cite{82} is written as:
\[
\frac{\partial}{\partial t} \gamma_{kk} + v \cdot \nabla \gamma_{kk} - \nabla v^T \cdot \gamma_{kk} - \gamma_{kk} \cdot \nabla v + \frac{1}{2\theta_k} \left( \gamma_{kk} \cdot \gamma_{kk} - \delta \frac{\Pi - I}{3} \gamma_{kk} \right) = 0
\] (3-120)

The velocity field for a one dimensional flow in cylindrical coordinates in a
tubular cavity is given by: \( u(r), v = w = 0 \). Thus, the velocity gradient is:
\[
\nabla v = \begin{vmatrix} 0 & 0 & \frac{\partial u}{\partial r} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{vmatrix} \quad \text{and} \quad \nabla v^T = \begin{vmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \frac{\partial u}{\partial r} & 0 & 0 \end{vmatrix}
\] (3-121)

The elastic strain tensor for one-dimensional tubular flow is written as:
\[
\gamma_{kk} = \begin{vmatrix} C_{rr,k} & 0 & C_{r,\theta,k} \\ 0 & 0 & 0 \\ C_{\theta,\theta,k} & 0 & C_{\theta,\theta,k} \end{vmatrix}
\] (3-122)

For Poiseuille flow in a tube, where no deformation in \( \theta \) direction is assumed, the
elastic tensor reduces to:
\[
\gamma_{kk} = \begin{vmatrix} C_{rr,k} & 0 & C_{r,\theta,k} \\ 0 & 1 & 0 \\ C_{\theta,\theta,k} & 0 & C_{\theta,\theta,k} \end{vmatrix}
\] (3-123)

One of the constraints for incompressibility for the Leonov model is that the
determinant of elastic strain tensor \( \gamma_{kk} \) is equal to unity. Thus, from Eq. (3-123) we have:
\[
\det \gamma_{kk} = C_{rr,k} C_{\theta,\theta,k} - C_{r,\theta,k}^T = 1
\] (3-124)

Calculating each term of Eq. (3-120)
The first and second invariants of tensor $C_{\kappa\kappa}$ (Eq. (3-123) are defined as:

\begin{align*}
I &= tr C_{\kappa\kappa} = C_{\nu,\kappa} + 1 + C_{\nu,\kappa} \quad (3-129) \\
II &= tr C^{-1}_{\kappa\kappa} = C_{\nu,\kappa} + C_{\nu,\kappa} C_{\nu,\kappa} - C_{\nu,\kappa}^2 + C_{\nu,\kappa} \quad (3-130) \\

\end{align*}

with

\begin{align*}
C^{-1}_{\kappa\kappa} &= \begin{vmatrix}
C_{\omega,\kappa} & C_{\nu,\kappa} & 0 & -C_{\nu,\kappa} C_{\omega,\kappa} \\
0 & C_{\nu,\kappa} & -C_{\nu,\kappa}^2 & 0 \\
-C_{\omega,\kappa} C_{\nu,\kappa} & 0 & C_{\nu,\kappa} & 0 \\
0 & C_{\nu,\kappa} & 0 & C_{\nu,\kappa}
\end{vmatrix} \\
(3-131)
\end{align*}

\begin{align*}
\nabla v \cdot C_{\kappa\kappa} &= \begin{vmatrix}
0 & 0 & 0 & C_{\nu,\kappa} & 0 & C_{\nu,\kappa} \\
0 & 0 & 0 & 0 & 1 & 0 \\
\frac{\partial u}{\partial r} & 0 & 0 & C_{\nu,\kappa} & 0 & C_{\nu,\kappa} \\
\frac{\partial u}{\partial r} & 0 & 0 & C_{\nu,\kappa} & 0 & \frac{\partial u}{\partial r} C_{\nu,\kappa}
\end{vmatrix} = \begin{vmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
\frac{\partial u}{\partial r} & 0 & 0 \\
\frac{\partial u}{\partial r} C_{\nu,\kappa}
\end{vmatrix} \quad (3-125)
\end{align*}

\begin{align*}
\frac{\partial u}{\partial r} C_{\nu,\kappa} &= \begin{vmatrix}
C_{\nu,\kappa} & 0 & C_{\nu,\kappa} & 0 & 0 & \frac{\partial u}{\partial r} \\
0 & 1 & 0 & 0 & 0 & 0 \\
C_{\nu,\kappa} & 0 & C_{\nu,\kappa} & 0 & 0 & 0 \\
0 & 0 & C_{\nu,\kappa} & 0 & \frac{\partial u}{\partial r}
\end{vmatrix} = \begin{vmatrix}
0 & 0 & C_{\nu,\kappa} & \frac{\partial u}{\partial r} \\
0 & 0 & 0 & \frac{\partial u}{\partial r}
\end{vmatrix} \quad (3-126)
\end{align*}

\begin{align*}
\frac{\partial u}{\partial r} C_{\nu,\kappa} &= \begin{vmatrix}
C_{\nu,\kappa} & 0 & C_{\nu,\kappa} & 0 & 0 & \frac{\partial u}{\partial r} \\
0 & 1 & 0 & 0 & 0 & 0 \\
C_{\nu,\kappa} & 0 & C_{\nu,\kappa} & 0 & 0 & 0 \\
0 & 0 & C_{\nu,\kappa} & 0 & \frac{\partial u}{\partial r}
\end{vmatrix} = \begin{vmatrix}
0 & 0 & C_{\nu,\kappa} & \frac{\partial u}{\partial r} \\
0 & 0 & 0 & \frac{\partial u}{\partial r}
\end{vmatrix} \quad (3-126)
\end{align*}

\begin{align*}
C \cdot C &= \begin{vmatrix}
C_{\nu,\kappa} & 0 & C_{\nu,\kappa} & 0 & C_{\nu,\kappa} \\
0 & 1 & 0 & 0 & 0 \\
C_{\nu,\kappa} & 0 & C_{\nu,\kappa} & 0 & C_{\nu,\kappa} \\
C_{\nu,\kappa} C_{\nu,\kappa} + C_{\nu,\kappa}^2 & 0 & C_{\nu,\kappa} C_{\nu,\kappa} + C_{\nu,\kappa}^2 & 0 & C_{\nu,\kappa} \\
C_{\nu,\kappa} C_{\nu,\kappa} + C_{\nu,\kappa}^2 & 0 & C_{\nu,\kappa} C_{\nu,\kappa} + C_{\nu,\kappa}^2 & 0 & C_{\nu,\kappa} \\
\end{vmatrix} \\
&= \begin{vmatrix}
C_{\nu,\kappa} C_{\nu,\kappa} + C_{\nu,\kappa}^2 & 0 & C_{\nu,\kappa} C_{\nu,\kappa} + C_{\nu,\kappa}^2 & 0 & C_{\nu,\kappa} \\
C_{\nu,\kappa} C_{\nu,\kappa} + C_{\nu,\kappa}^2 & 0 & C_{\nu,\kappa} C_{\nu,\kappa} + C_{\nu,\kappa}^2 & 0 & C_{\nu,\kappa} \\
\end{vmatrix} \quad (3-127)
\end{align*}

\begin{align*}
v \cdot \nabla C_{\kappa\kappa} &= u \frac{\partial}{\partial z} C_{\kappa\kappa} \quad (3-128)
\end{align*}
Substitution of Eq. (3-124) into Eq. (3-130) yields that the second invariant of the elastic strain tensor (Eq. (3-130)) becomes equal to its first invariant (Eq. (3-129)). Thus Eq. (3-120) can be rewritten as:

\[
\frac{\partial}{\partial t} C_{\kappa,k} + \nu \cdot \nabla C_{\kappa,k} - \nabla v^\prime \cdot C_{\kappa,k} - C_{\kappa,k} \cdot \nabla v + \frac{1}{2\theta_k} (C_{\kappa,k} \cdot C_{\kappa,k} - \delta) = 0
\]  

(3-132)

Substituting Eqs. (3-125 to 3-128) in Eq. (3-132) the governing equations for the \( k \)th mode for the strain tensor are:

\[
\frac{D}{Dt} C_{\kappa,k} = -\frac{1}{2\theta_k} (C_{\kappa,k}^2 + C_{\kappa,k}^2 - 1)
\]  

(3-133)

\[
\frac{D}{Dt} C_{\kappa,k} = \frac{\partial u}{\partial r} C_{\kappa,k} - \frac{1}{2\theta_k} (C_{\kappa,k} (C_{\kappa,k} + C_{\kappa,k}))
\]  

(3-134)

\[
\frac{D}{Dt} C_{\kappa,k} = 2 \frac{\partial u}{\partial r} C_{\kappa,k} - \frac{1}{2\theta_k} (C_{\kappa,k}^2 + C_{\kappa,k}^2 - 1)
\]  

(3-135)

Calculating the determinant of tensor \( C \) we have:

\[
C_{\kappa,k} C_{\kappa,k} = 1 + C_{\kappa,k}^2
\]  

(3-136)

The initial conditions for the elastic strain tensor at \( t = 0 \) are:

\[
C_{\kappa,k} (r,0) = 1; \quad C_{\kappa,k} (r,0) = 0; \quad C_{\kappa,k} (r,0) = 1
\]  

(3-137)

The steady state solution of the elastic strain tensor components are expressed as:

\[
C_{\kappa,k} = \frac{\sqrt{2X_k}}{\sqrt{1+X_k}}
\]  

(3-138)

\[
C_{\kappa,k} = \frac{2\gamma \theta_k}{1+X_k}
\]  

(3-139)
\[
C_{r,k} = \frac{\sqrt{2}}{\sqrt{1 + X_k}} \tag{3-140}
\]

where \( X_k = \sqrt{1 + 4(\dot{\gamma}\theta_k)^2} \), and \( \dot{\gamma} = \frac{\partial u}{\partial r} \) \tag{3-141}

To take into consideration the dependence of the material functions on temperature, the method of reduced variables is used [68]. The temperature-dependence of viscosity and relaxation time can be expressed by the WLF type as:

\[
\eta_k(T) = \eta_k(T_r) \cdot \frac{a_r}{a_{r_r}} \tag{3-142}
\]

\[
\theta_k(T) = \theta_k(T_r) \cdot \frac{a_r}{a_{r_r}} \tag{3-143}
\]

where \( a_r = \begin{cases}
\frac{a_{r_g}}{\exp \left[ -\frac{C_1(T - T_r)}{C_2 + T - T_r} \right]} & \text{if } T \leq T_g \\
\frac{a_{r_g}}{\exp \left[ -\frac{C_1(T - T_r)}{C_2 + T - T_r} \right]} & \text{if } T > T_g
\end{cases} \) is the shift factor; \( T_r \), the reference temperature selected depending on the polymeric material; and \( C_1 \) and \( C_2 \) are constants depending on the reference temperature.

3.7 Flow-Induced Stress Relaxation

The residual flow induced stresses are directly related with the flow history and the rheological properties of the polymer. When the polymer melt starts to solidify and reaches the glass transition temperature, the molecules lose their fluidity and the recoverable strain and stresses developed during the filling and packing may freeze, remaining then in the polymeric part as frozen-in residual stresses.
After the flow cessation the shear rate and velocity terms vanish,
\[ \dot{\gamma} = \frac{\partial u}{\partial r} = u(r) = 0. \]
So, making use of Eq. (3-119), the evolution equations for the elastic strain tensor (Eqs. (3-133) to (3-135)) take the form:

\[
\frac{d}{dt} C_{r,K} = -\frac{1}{2\theta_k}(C_{r,K} C_{r,K} + C_{z,K}) - 1 \quad (3-144)
\]

\[
\frac{d}{dt} C_{r,z} = -\frac{1}{2\theta_k}(C_{r,z} C_{r,z} + C_{z,z}) - 1 \quad (3-145)
\]

The initial conditions to calculate the elastic strain tensor during the stress relaxation Eqs. (3-144) to (3-146) are:

\[
C \bigg|_{t=0} = C \bigg|_{t,1} \quad (3-147)
\]

where \( t_s \) is the shearing time prior to flow cessation and the elastic strain tensor \( C \bigg|_{t,1} \) is the one that exists when the gas penetration is completed.

To calculate the birefringence components during the polymer flow, the stress-optical rule is employed yielding the following equations:

\[
\Delta n^f = \Delta n_{r,c}^f = C_f \left[ (\sigma_{rr} - \sigma_{zz})^2 + 4\tau_{r_z}^2 \right]^{1/2} \quad (3-148)
\]

\[
n_{rr}^f - n_{\theta\theta}^f = C_f (\sigma_{rr} - \sigma_{\theta\theta}) \quad (3-149)
\]

\[
n_{\theta\theta}^f - n_{zz}^f = C_f (\sigma_{\theta\theta} - \sigma_{zz}) \quad (3-150)
\]

where the superscript \( f \) indicates flow-induced birefringence components, \( C_f \) is the temperature dependent stress-optical coefficient of the polymer in melt state, \( \Delta n, n_{rr} - n_{\theta\theta} \).
and \( n_{zz} - n_{\theta\theta} \) are the birefringence components in the planes \( z-r, \theta-r \) and \( \theta-z \), respectively. 

\( \sigma_{ii} \) \((i = z, \theta, r)\) are the normal stresses in the \( z, \theta \) and \( r \) directions, respectively, and \( \tau_{rz} \) is the shear stress in the \( z-r \) plane.

3.8 Numerical Implementation

The governing equations for one dimensional tubular flow are given by Eqs. (3-101) to (3-106) for pressure and interface evolution, and by Eq. (3-21) for temperature distribution. The equations for pressure and interface evolution are coupled with the viscosity function of the polymer (Eq. (3-40)), which depends on the shear rate and the elastic strain tensor \( C_{ik} \). The evolution equation of the elastic strain tensor is a function of temperature and shear rate (Eqs.(3-133) to (3-135)). Therefore, the primary governing equations for the GAIM process is a set of highly non-linear equations that are solved using a numerical scheme. In the present formulation, the finite-element/control-volume/finite-difference (FE/CV/FD) approach developed by Winslow [117] and implemented by Li and Isayev [49, 115] is employed.

3.9 Pressure and Interface Development

To solve the pressure and interface evolution equations, the cylindrical mold cavity is discretized into a series of one-dimensional two-node tubular elements in the length-wise direction. The radial direction of each node is divided into equally spaced meshes to solve the temperature field by means of the finite-difference method. According to the Control-Volume method, a control volume is associated with each node in the length direction. The control volume is divided into two subcontrol volumes that
correspond to half of the volume of the adjacent elements. For the end nodes, the control volume is composed of one subcontrol volume that corresponds to half of the volume of the element associated with the end node. Fig. (3-1) shows a schematic diagram of the control volume representation for a node \(i\).

The pressure and the interface distribution on each element can be approximated using the nodal pressure and nodal interface positions by means of the linear interpolation functions, which are written as:

\[
p(z,t) = \sum_{j=1}^{2} L_j'(z)p_j'(t) \tag{3-151}
\]

\[
\delta(z,t) = \sum_{j=1}^{2} L_j'(z)\delta_j'(t) \tag{3-152}
\]
where $p'_j(t)$ and $\delta'_j(t)$ denote the nodal pressures and nodal interface positions, respectively, and $L'_j(z)$ denotes the linear interpolation functions and $j$ represents the global nodal coordinate.

For a one dimensional tubular element the linear interpolation functions are defined as:

$$L'_m = \frac{1}{\Delta l} (a_m + b_m z) \quad m = 1, 2$$

(3-153)

where $m$ is the local nodal coordinate of element $l$; $\Delta l$ is the length of the element $l$ which, in terms of the nodal coordinate system, is written as:

$$\Delta l = z_2 - z_1$$

(3-154)

and $a_m$ and $b_m$ for $m = 1, 2$ are:

$$\begin{bmatrix} a_1 & b_1 \\ a_2 & b_2 \end{bmatrix} = \begin{bmatrix} z_2 & -1 \\ -z_1 & 1 \end{bmatrix}$$

(3-155)

Based on the control volume approach, with the use of the finite-difference representation for the time derivative [117], Eqs. (3-55) or (3-113) and (3-109) or (3-111) can be discretized as follows [115]:

Pressure equation

$$\sum_{j=1}^{ku} \sum_{i=1}^{2} \left[ \frac{p^{k+1}_j - p^k_j}{\Delta t} G^i_j \overline{A^i} + S^i_j \overline{B^i} p^k_j + \overline{A^j} \right] = Q_i$$

(3-156)

Interface evolution equation

$$\sum_{j=1}^{ku} \sum_{i=1}^{2} \frac{d\delta^2_j}{dt} \cdot \overline{D^i}_j + \sum_{j=1}^{ku} \sum_{i=1}^{2} S^i_{gas} \overline{B^i}_j p_N^k = Q_{i, gas}$$

(3-157)
where $Q_i$ is the total volumetric flow rate for each node at any instant for the whole cavity domain; $Q_{i, gas}$ is the volumetric flow rate of the gas injected; $A_l$ denotes the area of element $l$ with the summation in $l$ being over all elements containing node $i$; $ku$ is the total number of elements containing node $i$; $p_N$ denotes the nodal pressure and $\delta_j$ denotes the nodal interface position at the start of the given time step. The matrices $B_{i,j}$ and $E_{i,j}$ are the influence coefficient of the nodal pressure to the net flow rate in element $l$ and the influence coefficient of the nodal volume change on the net flow rate in element $l$, respectively, which are written as:

$$B_{i,j} = \frac{\pi}{\Delta l} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$  \hspace{1cm} (3-158)

and

$$E_{i,j} = \begin{bmatrix} 2 & 1 \\ \frac{3}{3} & \frac{3}{3} \\ 1 & 2 \\ \frac{3}{3} & \frac{3}{3} \end{bmatrix}$$  \hspace{1cm} (3-159)

$D_{i,j}$ is the influence coefficient of the nodal interface location on the net flow rate in element $l$ and is written as:

$$D_{i,j} = \begin{bmatrix} 1 & 1 \\ \frac{2}{6} & \frac{6}{6} \\ \frac{1}{1} & \frac{1}{2} \\ \frac{6}{6} & \frac{2}{2} \end{bmatrix}$$  \hspace{1cm} (3-160)

The numerical solution of the equations to simulate the GAIM process was carried out in a simulation code written in FORTRAN programming language. The total cavity
length was discretized into 216 nodes and the radial direction at each node was
discretized into 99 equally spaced divisions.

3.10 Discretization of the Evolution Equation of the Leonov Model

To compute the flow-induced stresses during the filling and gas penetration
stages, the elastic strain tensor $C_K$ of the Leonov model has to be determined for each
time step and for all relaxation modes. Therefore, the governing equations of the elastic
strain tensor for one-dimensional tubular flow, Eqs. (3-133) to (3-135), were discretized
using a Finite-Difference approach. Time derivatives were discretized using forward
difference and space variables were discretized using backward difference at time $t = t + \Delta t$
[118]. The resulting discretized equations are:

$$
C_{zzK(i,j),i}^{k+1} - C_{zzK(i,j),i}^k + v_{zzK(i,j),i}^{k+1} \frac{\Delta t}{\Delta z} \left( C_{zzK(i,j),i}^{k+1} - C_{zzK(i-1,j),i}^{k+1} \right) - \\
2\Delta t \gamma_{K(i,j)}^{k+1} C_{zzK(i,j),i}^{k+1} + \frac{\Delta t}{2\theta_K} \left( (C_{zzK(i,j),i}^{k+1})^2 + (C_{zzK(i,j),i}^{k+1})^2 - 1 \right) = 0 
$$

(3-161)

$$
C_{rrK(i,j),i}^{k+1} - C_{rrK(i,j),i}^k + v_{rrK(i,j),i}^{k+1} \frac{\Delta t}{\Delta z} \left( C_{rrK(i,j),i}^{k+1} - C_{rrK(i-1,j),i}^{k+1} \right) - \\
\Delta t \gamma_{K(i,j)}^{k+1} C_{rrK(i,j),i}^{k+1} + \frac{\Delta t}{2\theta_K} \left( C_{rrK(i,j),i}^{k+1} \left( C_{rrK(i,j),i}^{k+1} + C_{zzK(i,j),i}^{k+1} \right) \right) = 0 
$$

(3-162)

$$
C_{rzK(i,j),i}^{k+1} - C_{rzK(i,j),i}^k + v_{rzK(i,j),i}^{k+1} \frac{\Delta t}{\Delta z} \left( C_{rzK(i,j),i}^{k+1} - C_{rzK(i-1,j),i}^{k+1} \right) + \\
\frac{\Delta t}{2\theta_K} \left( (C_{rzK(i,j),i}^{k+1})^2 + (C_{rzK(i,j),i}^{k+1})^2 - 1 \right) = 0 
$$

(3-163)

Where the superscript $k$ represents the time step and the subscript $K$ indicates the mode
number, $\theta_K$ is the $K^{th}$ relaxation time; $\Delta t$ is the time step; $C_{r,j,K}^t$ represents the components
of the elastic strain tensor in the Leonov model; \( u \) is the velocity component in the flow direction at node \( i \) and at radial position \( j \); and \( \gamma_{i,j}^{r} \) represents the shear rate \( \frac{\partial u}{\partial r} \).

Then, the components of the strain tensor were found solving the discretized system of equations (Eqs. (3-161) to (3-163)) by implementing the Globally Convergent Method for Nonlinear Systems of Equations [119]. This method is powerful but the numerical computation of the Jacobian matrix represents a disadvantage [119]. However, for this case the Jacobian matrix is available analytically. So the subroutine “fdjac” which calculate the Jacobian matrix numerically, was replaced by a function that provides the Jacobian calculated analytically. Thus, taking the derivatives of these equations with respect the variables \( C_{r,r,K(i,j)}^{k+1}, C_{r,z,K(i,j)}^{k+1} \) and \( C_{z,z,K(i,j)}^{k+1} \), we obtain the Jacobian matrix:

\[
\begin{bmatrix}
1 + \frac{\Delta t}{\Delta z} v_{z(i,j)}^{k+1} + \frac{\Delta t}{\theta_k} C_{z,K(i,j)}^{k+1} & -2\Delta t \gamma_{r,i,j}^{k+1} + \frac{\Delta t}{\theta_k} C_{r,r,K(i,j)}^{k+1} & 0 \\
\frac{\Delta t}{2\theta_k} C_{r,z,K(i,j)}^{k+1} & 1 + \frac{\Delta t}{\Delta z} v_{z(i,j)}^{k+1} + \frac{\Delta t}{2\theta_k} C_{r,r,K(i,j)}^{k+1} & -\Delta t \gamma_{r,z,i,j}^{k+1} + \frac{\Delta t}{\theta_k} C_{r,z,K(i,j)}^{k+1} \\
0 & \frac{\Delta t}{\theta_k} C_{r,z,K(i,j)}^{k+1} & 1 + \frac{\Delta t}{\Delta z} v_{z(i,j)}^{k+1} + \frac{\Delta t}{\theta_k} C_{r,z,K(i,j)}^{k+1}
\end{bmatrix} = 0 \tag{3-164}
\]

It is very important to notice that in Eqs. (3-161) to (3-164) the velocity component and the shear rate are not known a priory. So, the calculation of the elastic strain tensor proceeds by iteration together with the subroutine that calculates the velocity and shear rate profiles. The latter values are updated each iteration in order to calculate the new \( C \) tensor until meet the convergence criteria. The iteration procedure is described later in the solution algorithm.
3.11 Temperature Distribution

The temperature distribution along the radius of the tubular molding is determined by solving the energy equation using a finite-difference method. For both, the polymer and gas domains, the energy equation for a one-dimensional tubular geometry reduces to:

\[ \rho_i c_{p,i} \left( \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial z} \right) = \frac{\kappa_i}{r} \frac{\partial T}{\partial r} + \kappa_i \frac{\partial^2 T}{\partial r^2} + \Phi_i, \]  

(3-165)

where \( i \) represents the polymer or gas domain; \( \rho_i \) is the density; \( C_{p,i} \) and \( \kappa_i \) are the specific heat and thermal conductivity, respectively; \( T \) is the temperature; \( u \) is the velocity in the flow direction, and \( \Phi_i \) is the dissipation term, which is neglected for the gas domain.

During the filling and primary gas penetration stages, the convective and dissipative terms in energy equation are considered. However, for the secondary gas penetration stage, where most of the cooling takes place and the velocity of gas is negligible, the convective and heat dissipation terms are neglected. Therefore, Eq. (3-165) reduces to a heat conduction problem:

\[ \rho_i C_{p,i} \frac{\partial T}{\partial t} = \frac{\kappa_{th,i}}{r} \frac{\partial T}{\partial r} + \kappa_{th,i} \frac{\partial^2 T}{\partial r^2} \]  

(3-166)

To solve the energy equation the boundary conditions given in Eqs. (3-26) and (3-27) are used. The solutions of Eqs. (3-165) and (3-166) give the temperature profile in the tubular molding. However, it can be noticed for the axisymetric cylindrical problem that these equations show an indetermination at the center line \( (r=0) \) where the temperature gradient vanishes \( (\partial T/\partial r = 0) \). Thus, using the L’Hospital rule on the first term on the right hand side of Eqs. (3-165) and (3-166) we obtain the energy equation that applies at the centerline for the filling and primary gas penetration stages:
\[ \rho c_p \left( \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial z} \right) = 2 \kappa_{m,j} \frac{\partial^2 T}{\partial r^2} + \Phi \]  

(3-167)

and for the secondary gas penetration stage:

\[ \rho c_p \left( \frac{\partial T}{\partial t} \right) = 2 \kappa_{m,j} \frac{\partial^2 T}{\partial r^2} \]  

(3-168)

Eq. (3-165) is solved following the procedure by Hieber and Shen [120] implemented by Li [95], in which, the radial direction of each control volume that forms the cavity is divided into a set of uniform meshes. Such that:

\[ T_{i,j}^k = T(z_i, r, t_k) \]  

(3-169)

where the subscripts \( n \) and \( j \) represent the discretization in flow and radial directions, respectively, and \( k \) represent the time step.

To calculate the convection term, \( u \frac{\partial T}{\partial z} \), during the filling and gas penetration stages, the temperature distribution in the flow direction, \( z \), is linearly interpolated within each element, \( l \), according to:

\[ T'_{j}(z, r, t) = \sum_{j=1}^{2} L_j'(z)T_j'(r, t) \]  

(3-170)

where \( L_j'(z) \) is the linear interpolation function for a tubular element given by Eq. (3-153).

To solve the energy equation, an implicit scheme is used where the transient \( (\partial T/\partial t) \) and conduction \( (\partial T/\partial z) \) terms of the energy equation are discretized using forward-difference and central-difference at \( t+\Delta t \), respectively [118], and the convection and viscous-heating terms are calculated at an earlier time. In the finite-element method, the pressure gradient, the velocity and shear rate are continuous functions within each
element but, these functions are discontinuous at each node [120]. To overcome this problem, a weighted average of the pressure gradient and the quantities associated with it are calculated based on the fractional volume contribution of each element associated with the node, \( i \).

The convective term is calculated at the centroide of each element and substitution of the interpolation function (Eq. (3-153)) into Eq. (3-170) and taking the derivative with respect to the flow direction, \( z \), we obtain the following expression:

\[
\frac{\partial T'(z,r,t)}{\partial z} = \sum_{m=1}^{\hat{m}} \frac{1}{\Delta l} b_m T'_w(r,t)
\]

(3-171)

The velocity at the centroide of each element is given by Eq. (3-86). Thus, the convective term at the centroide of each element results in:

\[
u' \frac{\partial T'(z,r,t)}{\partial z} = \frac{\partial p'}{\partial z} \frac{1}{2} \frac{r'}{\eta'} \int_{r'}^r dr' \left[ \sum_{m=1}^{\hat{m}} \frac{1}{\Delta l} b_m T'_w(r,t) \right]
\]

(3-172)

Making use of equation (3-75) and taking the weighted average of the fractional contribution of each sub-control volume, we obtain the equation for the convective term at each node written as:

\[
\frac{1}{\sigma_{i,k}} \sum_{i,j} \theta^i_{j,k} \nu' \frac{\partial T'(z,r,t)}{\partial z} = \frac{1}{\sigma_i} \sum_{i,j} \theta^i_{j,k} \frac{\partial p'}{\partial z} \gamma' \int_{r'}^r dr' \sum_{m=1}^{\hat{m}} \frac{1}{\Delta l} b_m T'_w(r,t)
\]

(3-173)

\( \theta^i_{j,k} \) is the fraction of control volume containing element \( l \) and

\[
\sigma_i = \sum_{l=1}^{\hat{k}} \theta^i_{j,k}
\]

(3-174)

where \( \sigma_i \) is the total control volume associated with each node.
Using a similar procedure to average the viscous heating term, the energy equation for each node, results in:

\[
\rho c_p \left( \frac{T^{k+1}_{i,j} - T^k_{i,j}}{\Delta t} + \frac{1}{\sigma_i} \sum_{l=1}^{kn} \theta_j^{il} \sum_{m=1}^{2} E_{i,m,j} \cdot T^k_{i,j} \right) = \frac{2 \kappa_{ij} (T^{k+1}_{i,j} - 2T^k_{i,j} + T^{k-1}_{i,j}) + \kappa_{ij} (T^k_{i,j} - T^{k+1}_{i,j}) + \Phi_{i,j}}{\Delta r^2} + \frac{k_{bj} (T^{k+1}_{i,j} - T^k_{i,j} + T^{k-1}_{i,j})}{2r_i \Delta r} + \Phi_{i,j}
\]  

(3-175)

with \( E_{m,i,j} = \frac{1}{\Delta l} \left( \frac{\partial p}{\partial z} \right)^{i,j} \int \frac{\partial p}{\partial z} \, dz (b_n) \)  

(3-176)

and the dissipation function at the nodal vertex is written as:

\[
\Phi^{i,j} = \frac{1}{\sigma_i} \sum_{l=1}^{kn} \theta_j^{il} \left( \Phi_j^{i} \right)
\]  

(3-177)

where

\[
\Phi_j^{i} = 2s \eta \text{tr}(e_j^{i}) + \sum_{k=1}^{K} \eta_x \frac{1}{4 \theta_x} \left[ \frac{1}{3} \text{tr} C_j^{i} - \text{tr} \left( C_j^{i} - 3 \epsilon_j^{i} \right) \right]
\]  

(3-178)

The dissipation function is a known quantity when the temperature is calculated in Eq. (3-175), since the deformation rate tensor \( (\varepsilon) \) and elastic strain tensor \( (\varepsilon) \) are calculated in the previous time step.

Eq. (3-175) is applicable for the polymer and gas domains at each node. However, it is indetermined at the centerline for the second term on the right hand side, which is solved by using Eq. (3-167) where L’Hospital’s rule has been applied to the heat conduction term. The discretized equation of the conduction term of Eq. (3-167) results:

\[
2 \kappa_{ij} \frac{\partial^2 T}{\partial r^2} = 2 \frac{\kappa_{ij} (T^{k+1}_{i,j} - 2T^k_{i,j} + T^{k-1}_{i,j})}{\Delta r^2} + \frac{k_{bj} (T^{k+1}_{i,j} - T^k_{i,j} + T^{k-1}_{i,j})}{2r_i \Delta r} + \Phi_{i,j}
\]  

(3-179)
Considering that the temperature profile is symmetric with respect to the center line, \( \frac{\partial T}{\partial r} = 0 \), then, the derivative is discretized using central-difference of second order which yields:

\[
T_{r,i,j}^{k+1} = T_{r,i,j-1}^{k+1}
\]  

(3-180)

Substitution of Eq. (3-180) into Eq. (3-179) reduces to:

\[
2\kappa_{db,i,j} \frac{\partial^2 T}{\partial r^2} = 4\kappa_{db,i,j} \left( T_{r,i+1}^{k+1} - T_{r,i}^{k+1} \right)
\]  

(3-181)

At the polymer/gas interface, the temperature and heat flux are considered continuous through the interface:

\[
T_{pol} \bigg|_i = T_{gas} \bigg|_i \quad \text{and} \quad \left( \kappa \frac{\partial T}{\partial r} \right)_{pol} = \left( \kappa \frac{\partial T}{\partial r} \right)_{gas}
\]  

(3-182)

The solution of Eq. (3-175) considering both, the gas and polymer domains is implemented using the successive under-relaxation method. The temperature at the entrance node is considered equal to the melt temperature (Eq. (3-23)), the temperature of the polymer in contact with the mold is considered equal as the mold temperature (Eq. (3-26)), and the temperature of the advancing melt front is determined according to the temperature of the previous melt front [84]. For tubular elements, the temperature of the advancing melt front reduces to:

\[
T_{r,i''}^k = \frac{T_{r,i+1}^k + T_{r,i-1}^k}{2}
\]  

(3-183)

where \( i'' \) represents the melt front node.
3.12 Melt Front Advancement

In the present formulation, a method similar to the Flow Analysis Network (FAN) [121] is employed. In this method, the filling parameter factors for the gas and polymer domains, respectively, $f_{\text{gas}}$ and $f_{\text{pol}}$, are associated with each control volume. These filling factors vary between 0 and 1 according to the fraction of the control volume occupied by the polymer during the filling stage, or by the polymer/gas ratio for the gas penetration stage. The entrance and intermediate nodes are assumed to be fully filled during the whole process, thus, the filling parameters are equal to 1. Both $f_{\text{gas}}$ and $f_{\text{pol}}$ vary between 0 and 1 depending on the degree of filling of the control volume. It is important to mention that the fountain flow effect at the advancing melt front is neglected in the present formulation. So, the advancing gas and melt fronts are assumed to be flat in the radial direction. At the melt front nodes, the net flow entering the control volume is computed from the volume flow rate coming from the fully filled adjacent nodes. The volume flow rate for a partially filled node is determined from Eq. (3-156) where the net flow rate, $Q_N$, is different from zero and the relative pressure at the melt front vanishes (atmospheric pressure). Physically, the total flow rate of the melt front nodes is equal to the net flow rate at the entrance node, this concept is used as a convergence criteria. The time increment is calculated assuming that only one partially filled node is filled during each time step.

During the calculations, the total flow rate at the melt front nodes may not be the same as the specified flow rate at the entrance nodes. Thus, the pressure is scaled in order to satisfy the continuity equation until convergence is reached. In the control volume
approach, the flow rate at the entrance node is calculated according to the average gapwise velocity at the centroid of the element.

Once the pressure has satisfied the convergence criteria, the velocity components are determined. The temperature profile for the next time is calculated taking into account the velocity and viscous heating terms. This procedure is repeated until the cavity is fully filled.

The filling parameter $f_{gas}$ for the gas domain is introduced to identify those nodes corresponding to the gas front in which $0 < f_{gas} < 1$, noting that $f_{pol} = 1 - f_{gas}$. For the interior nodes in the gas domain, $f_{gas} = 1$ and $f_{pol} = 0$. Consequently, for the interior nodes in the polymer domain where the gas has not penetrated, the filling parameters are: $f_{gas} = 0$ and $f_{pol} = 1$. The time interval is determined considering that only one control volume either in the gas or polymer domains is filled per each time step. The volume of fluid method (VOF) [122] is used to track the gas and polymer melt front advancement. In the VOF method, the degree of filling of each control volume is specified by the volume of fluid function $F$, which is governed by:

$$\frac{\partial F}{\partial t} + \vec{V} \nabla F = 0$$

(3-184)

where $F$ represents the filling factor, and $\vec{V}$ the velocity vector.

The advection of the fluid volume is based on the conservation of mass on each control volume. The conservation of mass on each control volume is related to the change of the filling factor of each melt front at each time step with the net flow rate of fluid into the control volume. Therefore:
\[ F_{n+1} = F_n + \Delta t \frac{\sum q_{n,j}}{V_n} \quad (3-185) \]

where \( V_n \) represent the total volume of the control-volume associated with node \( i \), and \( q_n \) is the net flow rate entering each subcontrol volume.

The filling factors of both the gas and polymer domains are updated each time step using Eq. (3-185). Thus, a new filled domain is defined and the melt front nodes are updated.

3.13 Solution Algorithm for GAIM

The solution of the governing equations for the filling phase is done in three main stages [84, 114]:

1. calculation of the pressure field and interface position;
2. calculation of the temperature field;
3. advancing of the flow front.

During the filling stage, the flow rate \( Q_i \) at the entrance node is determined by the injection speed at which the polymer is delivered into the mold. The polymer melt temperature at the injection point is taken as the injection temperature and the pressure at the flow front is neglected. In the first time step, a pressure gradient is assumed, and using the steady state solution of the elastic strain tensor \( C \) (Eqs. (3-138) to (3-141)) the shear rate is calculated iteratively using Eqs. (3-39) and (3-40) which are rewritten as follows [108]:

\[ \frac{\partial u_{m+1}}{\partial r} = \frac{\partial p}{\partial z} \frac{r}{2\eta_2} \quad (3-186) \]
with

$$\eta_\varepsilon^m = \eta_s + \sum_{k=1}^{N} \frac{\eta_s C_{r,\kappa}^m \partial u^m}{\partial r}$$

(3-187)

where \( m \) is the iteration number.

It can be observed that at convergence, \( \frac{\partial u^{m+1}}{\partial r} = \frac{\partial u^m}{\partial r} \), Eqs. (3-186) and (3-187) reduce to the original Leonov equation.

Once the shear rate is obtained, the fluidity \( S \) is calculated using Eq. (3-48). Then, the volume flow rate is calculated solving the pressure equation (Eqs. (3-47)) by means of the control-volume/finite-element approach. This equation is solved using the boundary conditions shown in Eqs. (3-28) and (3-29), and the elastic strain tensor. The calculated volume flow rate is compared with the specified volume flow rate at the entrance node. The pressure is assumed to converge when the absolute difference between the calculated and specified flow rates reaches a specified convergence criteria. If the convergence criterion is not satisfied, the calculation is performed again, updating the pressure using the under-relaxation method [84]:

$$p = (1 - \omega) p_{\text{old}} + \omega p_{\text{new}}$$

(3-188)

where \( \omega \) is the under-relaxation parameter lying between 0 and 1, and \( p_{\text{old}} \) and \( p_{\text{new}} \) denote the pressure at the previous and present iteration, respectively.

Once the pressure has converged, the velocity components are determined, and the temperature field is resolved using Eq. (3-175). The temperature profile for time \( t_2 = t_1 + \Delta t \) is calculated based on the velocity and viscous heating at time \( t_1 \). This procedure
is continued until the specified volume of polymer melt (shot size) inside the cavity is
reached.

After the polymer has been introduced into the mold cavity, the gas is injected at
constant pressure at the entrance node (Eq. (3-29)). To solve the governing equations of
the primary gas penetration, the pressure and interface evolution equations (Eqs. (3-156)
and (3-157)) have to be solved simultaneously [115]. In the present implementation,
successive under-relaxation is employed for the pressure field and the calculation
proceeds in the same way as in the filling stage.

During the cooling stage, the stress relaxation is governed by Eqs. (3-133) to (3-136).
In this stage, the dissipation and conduction terms vanish and Eq. (3-175) reduces to a
heat conduction problem.

With the shear rate and temperature profiles determined for each filled node, the
physical quantities of the polymer such as density change, shear stresses, first and second
normal stress differences, flow-induced birefringence and interface distribution can be
tracked throughout the simulation of the GAIM process.

Fig. 3-2 shows the flow chart of the solution of the GAIM process.
Figure 3-2 Flow chart of the solution of the GAIM simulation
Figure 3-2 Flow chart of the solution of the GAIM simulation (Continued).

A

Calculate the melt front advancement

Calculate the temperature field

Calculate the flow induced stress and birefringence

Write the transient results at specific nodes

Update the filling factors for the newly filled nodes and calculate the next time step

B

Cavity filled & polymer temperature is below $t_g$?

No

Yes

Write final results

End program

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CHAPTER IV
MODELING OF THERMALLY-INDUCED STRESSES AND BIREFRINGENCE

Thermal stresses occur in parts that experience inhomogeneous temperature variations. In the case of elastic materials subjected to free thermal expansion, a temperature gradient induces transient thermal stresses that vanish when the sample reaches a homogeneous final temperature. This ideal process occurs only if there is no plastic deformation and the material properties throughout the sample are homogeneous at the initial and final states [123, 124]. Thermally-induced residual stresses arise due to the combination of an inhomogeneous temperature distribution and a strong dependence of the material’s mechanical properties on temperature. In the case of polymeric materials, owing to their low thermal conductivity, the cooling process generates a large temperature gradient and each position along the sample thickness reaches a final temperature at different times. As a consequence, each point experiences different thermal history. During the cooling process, due to the temperature gradient, the polymer contracts at different proportion causing thermal stresses. These stresses partially relax in those regions where the temperature is elevated. However, when the polymer cools down from above to below the glass transition temperature, its Young’s modulus increases several orders of magnitude [125]. Therefore, the part of the thermal stresses generated
during solidification will not relax resulting in residual stress distribution in the final product [124].

There are several techniques to measure the residual stresses in polymeric articles. A review of these techniques is found elsewhere [124]. The best known technique to determine the residual stresses, is the layer-removal method developed by Treuting and Read [126]. This method works well for certain materials but it has some difficulties when it’s applied to polymers [127], in particular, measuring the curvature of the removed layer. One alternative that offer an excellent spatial resolution and high measurement accuracy is the birefringence method. The components of the residual birefringence reflect the state of stresses in the sample. However, the correlation of the residual birefringence with the thermally-induced residual stresses is not straightforward since the birefringence depends on the thermal history and not just on the final state of residual stresses. Nevertheless, the relative ease with which the birefringence is measured in transparent polymers, worth the effort to attempt a qualitative determination.

This chapter presents the mathematical derivation to calculate the thermally-induced stresses and birefringence generated during free quenching of viscoelastic tubes and rods. The formulation was confined to a quasi-static analysis with the hypothesis of infinitesimal deformations of linear viscoelastic cylindrical bodies that experience temperature changes only along the radius. The ends and free surfaces of the tubes and rods are assumed free of any force. The cylindrical body is assumed to be free of stresses and birefringence at the initial temperature, and to remain in plane strain condition during the quenching process.
4.1 Calculation of the Temperature Distribution in Free Quenching

The temperature distribution of the cylinder was calculated using the energy equation (Eq. (3-3)). In the present simulation, it is assumed that the temperature varies only along the radius and there is no thermodynamical coupling. As a consequence, the viscous heating and convective terms of the energy equation vanish, yielding:

$$\rho C_p \left( \frac{\partial T}{\partial t} \right) = \frac{\kappa}{r} \frac{\partial T}{\partial r} + \kappa \frac{\partial^2 T}{\partial r^2}$$

(Eq. 4-1)

Eq. (4-1) was solved numerically using the Crank-Nicolson method [128]. During the quenching experiments, the external surface of the tubes and rods was in contact with water. Therefore, a convective boundary condition was imposed at the external surface, given by:

$$-h(T_s - T_f) = \kappa \frac{\partial T}{\partial r}$$

(Eq. 4-2)

where $h$ is the heat transfer coefficient, $T_s$ is the temperature at the temperature of the surface of the tube or rod, $T_f$ is the fluid’s temperature, and $\kappa$ is polymer’s thermal conductivity.

In the case of tubes, the boundary condition at the tube’s inner wall was considered adiabatic, i.e. $\frac{\partial T}{\partial r} = 0$. This assumption could be made since the air inside the tube was confined during the quenching experiments. Furthermore, this air was at atmospheric pressure and its density is roughly three orders of magnitude lower than the polymer’s density. Therefore, the air’s volumetric heat capacity ($\rho C_p$) is very low compared with that of the polymer. Consequently, the heat stored by the air compared to that stored by the polymer can be considered negligible for practical purposes [129].
In the case of rods the boundary condition at the center is given by the symmetry condition. To avoid the indetermination at the centerline, the L’Hospital rule was employed, as described in Section 3.11.

4.2 Thermally-Induced Residual Stress and Birefringence

Several approaches have been developed to calculate the thermally-induced residual stresses in polymers [9, 11, 97, 98, 104, 111, 130]. The approach employed in this work is the linear viscoelastic theory proposed by Morland and Lee [9]. The use of a linear viscoelastic constitutive equation to calculate the stresses generated during cooling is due to the fact that the polymer behaves totally different at temperatures above and below \( T_g \). Below \( T_g \), it is assumed that the polymer does not flow and the thermal strains are small and are linearly proportional to the stresses. The Morland and Lee theory takes into account the relaxation modulus with respect to time considering the mechanical response of the material as linear viscoelastic. The constitutive equation proposed by Morland and Lee for thermorheologically simple materials is written as follows:

\[
\sigma_{ij}(t) = \int_0^t 2G(t - \tau) \frac{\partial}{\partial \tau} \left[ \varepsilon_{ij} - \frac{1}{3} \varepsilon \delta_{ij} \right] d\tau + \varepsilon \delta_{ij} \int_0^t 2K(t - \tau) \frac{\partial}{\partial \tau} [I_{\varepsilon}] d\tau \tag{4-3}
\]

where \( \sigma_{ij} \) is the stress tensor, \( G \) and \( K \) are the time-dependent shear and bulk modulus, respectively, \( \varepsilon_{ij} \) is the strain tensor, \( \delta_{ij} \) is the unit tensor, and \( I_{\varepsilon} \) is the volume expansion which, in terms of the strain components, is defined as:

\[
I_{\varepsilon} = Tr(\varepsilon) = \varepsilon_{rr} + \varepsilon_{\theta\theta} + \varepsilon_{zz} \tag{4-4}
\]

where \( \varepsilon_{rr}, \varepsilon_{\theta\theta}, \) and \( \varepsilon_{zz} \) are the strains in \( r, \theta, \) and \( z \) directions respectively.
The two terms on the right hand side of Eq. (4-3) represent the deviatoric and dilatational responses of the viscoelastic material with respect to the elapsed time \((t-\tau)\). Accordingly, there is a possibility that two distinct shift functions govern the temperature-dependent shear and dilatation responses. This possibility is excluded since for thermorheologically simple materials, “the relaxation modulus in tension displays the shift property if, and only if, the two shift functions just mentioned are identical” [131].

The birefringence in polymers is dependent on the thermo-mechanical history that the material experienced during processing. The refractive index tensor completely determines the birefringence and it depends on the history of deformation which is described by the strain tensor. The constitutive equation to calculate the refraction index tensor in polymers under small deformations is given by [10, 132]:

\[
\int_{\epsilon} n_{ij}(t) = n_{ij}^0 + \int_0^t C_{\epsilon}(t-\tau) \frac{\partial}{\partial \tau} \left[ \epsilon_{ij} - \frac{1}{3} \epsilon_{kk} \delta_{ij} \right] d\tau + \int_0^t \Delta_{\epsilon}(t-\tau) \frac{\partial}{\partial \tau} \left[ I_{\epsilon} \right] d\tau
\]

(4-5)

where \( n_{ij} \) is the refraction tensor, \( n_0 \) is the initial birefringence, \( C_\epsilon \) is the strain-optical coefficient, \( \Delta_\epsilon \) is the bulk strain-optical coefficient, \( \epsilon_{ij} \) is the strain tensor, \( \epsilon_{kk} \) is the volume expansion.

To calculate the thermal strain history, the volume relaxation approach was considered [133]. This theory states that when the polymer is quenched from an initial temperature higher than \( T_g \) to an equilibrium temperature lower than \( T_g \), the polymer does not contract immediately. The contraction can be considered to happen in two steps: an instantaneous contraction followed by a gradual contraction to the equilibrium volume. The instantaneous contraction is assumed to be due to the reduction of the occupied volume, while the gradual contraction is assumed to be due to the relaxation of the free
volume to reach its equilibrium state. The reason because the free volume does not attain its equilibrium state immediately, is because at low temperatures, the contraction of the free volume (or the motion of the molecules) takes time to accomplish. Therefore, it is assumed that the polymer’s free volume relaxation follows the first-order-rate equation which, in terms of linear thermal strain, is written as [104]:

$$\frac{d\varepsilon_T}{dt} = \beta_s \frac{dT}{dt} - \frac{\varepsilon_T - \varepsilon_{Te}}{\theta_a T}$$

(4-6)

where \(\varepsilon_T\) and \(\varepsilon_{Te}\) are the actual and equilibrium thermal strain at the current temperature \(T\), \(\theta_a\) is the relaxation time at the reference temperature \(T_r\), \(a_T\) is the shift factor and \(\beta_g\) is the linear thermal expansion coefficient in the glassy state.

The equilibrium thermal strain is given by:

$$\varepsilon_{Te} = \begin{cases} 
\beta_l (T - T_i) & \text{if } T > T_2 \\
\beta_l (T_2 - T_i) + \beta_g (T - T_2) & \text{if } T < T_2 
\end{cases}$$

(4-7)

where \(\beta_l\) and \(\beta_g\) are the linear thermal expansion coefficient at the rubbery and glassy states, respectively, \(T_i\) is the initial temperature, and \(T_2\) is the secondary glass transition temperature where the free volume and conformational entropy become zero.

Polymers exhibit both, time- and temperature-dependent mechanical properties, and many polymers obey the time-temperature superposition principle proposed by Leaderman [99]. This principle states that for a constant change of temperature, a pure shift in relaxation modulus, viscosity, and other characteristic functions of the material is observed. Then, the shift factor, \(a_T\), can be obtained with the Williams-Landel-Ferry (WLF) equation which can be written as:
\[ \log a_T = -\frac{B(T - T_r)}{\alpha_f (T_r - T_2)(T_r - T_2) + T - T_r} \]  

(4-8)

where \( a_T \) is the shift factor, \( \alpha_f \) is the thermal expansion coefficient of the fractional free volume above \( T_2 \), \( T \) and \( T_r \) are the temperature and reference temperature, respectively.

If we make:

\[ C_1 = \frac{B}{\alpha_f (T_r - T_2)} \]  

(4-9)

and

\[ C_2 = (T_r - T_2) \]  

(4-10)

Eq. (4-8) becomes similar to the WLF equation which is valid for polymer melts between \( T_g \) to \( T_g + 100 \) °C. The constants \( C_1 \) and \( C_2 \) were evaluated by fitting the WLF equation to the data above the glass transition temperature. Once these constants were obtained \( T_2 \) and \( B \) were calculated from Eqs. (4-9) and (4-10). At temperatures below \( T_g \) the WLF equation cannot describe the polymer’s relaxation behavior in the glassy region. To overcome this problem, Rusch [133] introduced the concept of “effective temperature” which is the temperature of an equilibrium state which has the same free volume as the current non-equilibrium state. Therefore, the shift factor function becomes:

\[ \log a_T = -\frac{B(T_{eff} - T_r)}{\alpha_f (T_r - T_2)(T_r - T_2) + T_{eff} - T_r} \]  

(4-11)

where \( T_{eff} \) is the effective temperature. \( T_{eff} \) is treated as a fitting parameter using the same constants \( C_1 \) and \( C_2 \) calculated for the WLF equation.

According to the time-temperature superposition principle, the polymer’s shear relaxation modulus, \( G \), after certain time, \( t \), and at a temperature, \( T \), corresponds to that at
a pseudo-time given by \( t/a_T(T) \) at the reference temperature, \( T_r \). The term \( t/a_T(T) \) is called the reduced time \( \xi \) and it is defined as:

\[
\xi = \frac{t}{a_T(T)}
\]  

(4-12)

In a non-isothermal process, the temperature field varies with time. Then, to include the time-dependent temperature field the following relation is introduced [134]:

\[
\xi(t) = \int_0^t \frac{dt'}{a_T(T)}
\]  

(4-13)

Replacing the time, \( t \), by the reduced time, \( \xi \), in Eqs. (4-3) and (4-5), we obtain the equations to calculate the stresses generated by the polymer’s thermal contraction and the refraction index tensor in terms of the reduced time, respectively [134]. They are written as:

\[
\sigma_{ij}^{\xi_m}(\xi_m(t)) = \int_0^{\xi_m} 2G(\xi_m - \xi_m') \frac{\partial}{\partial \xi_m} \left[ \varepsilon_{ij}(\xi_m') - \frac{1}{3} \varepsilon(\xi_m') \delta_{ij} \right] d\xi_m' + \Delta \int_0^{\xi_m} K(\xi_m - \xi_m') \frac{\partial}{\partial \xi_m} \left[ \varepsilon(\xi_m') - 3 \varepsilon(\xi_m') \delta_{ij} \right] d\xi_m'
\]  

(4-14)

\[
n_{ij}^{\xi_C}(\xi_C(t)) = n_0 \delta_{ij} + \int_0^{\xi_C} C_e(\xi_C - \xi_C') \frac{\partial}{\partial \xi_C} \left[ \varepsilon_{ij}(\xi_C') - \frac{1}{3} \varepsilon(\xi_C') \delta_{ij} \right] d\xi_C' + \Delta \int_0^{\xi_C} \Delta_e(\xi_C - \xi_C') \frac{\partial}{\partial \xi_C} \left[ \varepsilon(\xi_C') - 3 \varepsilon(\xi_C') \delta_{ij} \right] d\xi_C'
\]  

(4-15)

where \( \xi_m \) is the reduced time for the modulus and \( \xi_C \) is the reduced time for the strain optical coefficient.

Eqs. (4-14) and (4-15) have different reduced times, \( \xi_m \) and \( \xi_C \), since the shift factor for the shear modulus and strain-optical coefficients may be different.
4.3 Thermal Stresses in Cylindrical Tubes and Rods

There are various methods to determine the thermal stresses in cylindrical bodies, one of the most common is the displacement technique [135]. In this method, the stress equilibrium equation is expressed in terms of strains by means of the stress-strain relations. In turn, the strains are expressed in terms of displacements by means of the strain-displacement relations. Consequently, the stress equilibrium equation is obtained in terms of displacements [136]. As a first approximation, the thermal stresses in free quenched tubes and rods are calculated assuming a plane strain condition in the axial direction.

For a quasi-static analysis, the inertial terms of the momentum equation are neglected and the equilibrium equation is considered instead [137]. Considering that the stress distribution is symmetrical with respect to the axial axis, \( z \), the stress components \( \sigma_{zz}, \sigma_{rr}, \) and \( \sigma_{\theta\theta} \), become independent of the axial and tangential directions. Furthermore, from symmetry, the shear stresses vanish. Therefore, the stress components \( \sigma_{zz}, \sigma_{rr}, \) and \( \sigma_{\theta\theta} \) are functions of the radius only and become the principal stresses during the loading history [123, 138]. The stress problem can be formulated as follows [139]:

\[
\begin{align*}
\sigma_{zz} &= \sigma_{r\theta} = \sigma_{\theta\theta} = 0 \\
\varepsilon_{zz} &= \varepsilon_{r\theta} = \varepsilon_{\theta\theta} = 0
\end{align*}
\]  

(4-16) (4-17)

The stress equilibrium equation in the radial direction is given by [123]:

\[
\frac{\partial \sigma_{rr}}{\partial r} + \frac{\sigma_{rr} - \sigma_{\theta\theta}}{r} = 0
\]  

(4-18)

where \( \sigma_{rr} \) and \( \sigma_{\theta\theta} \) are the radial and circumferential stresses, respectively.
The strain-displacement relations in cylindrical coordinates in radial, circumferential, and axial directions are:

\[ \varepsilon_{rr} = \frac{\partial u_r}{\partial r} \]  
(4-19)

\[ \varepsilon_{\theta\theta} = \frac{u_r}{r} \]  
(4-20)

\[ \varepsilon_{zz} = \frac{\partial u_z}{\partial z} \]  
(4-21)

where \( \varepsilon_{rr}, \varepsilon_{\theta\theta}, \) and \( \varepsilon_{zz}, \) are the strains in \( r, \theta, \) and \( z \) directions respectively, and \( u_r \) and \( u_z \) are the displacements in the radial and axial direction, respectively.

For the free quenching problem, it is considered that both ends and the curved surfaces of the cylindrical body are free of any traction. Furthermore, for the plane strain approximation, the stability condition states that the axial forces distribution in the plane \( r-\theta \) is in equilibrium. Then, the compressive and tensile regions of the axial stresses distribution along the radius are balanced. Accordingly, this condition is given by:

\[ 2\pi \int_a^b \sigma_{zz} r dr = 0 \]  
(4-22)

where integration limits, \( a \) and \( b \), represent the inner and outer radius of the cylinder, respectively. In the case of rods, the inner radius vanishes, i.e. \( a=0 \).

Expanding Eq. (4-14) we obtain:

\[
\left| \begin{array}{ccc}
\sigma_{rr} & \tau_{r\theta} & \tau_{rr} \\
\tau_{\theta\theta} & \sigma_{\theta\theta} & \tau_{r\theta} \\
\tau_{rr} & \tau_{r\theta} & \sigma_{zz}
\end{array} \right| = \int_0^{\xi_m} 2G(\xi_m - \xi') \frac{\partial}{\partial \xi_m} \left[ \begin{array}{ccc}
\varepsilon_{rr} & \varepsilon_{r\theta} & \varepsilon_{rr} \\
\varepsilon_{\theta\theta} & \varepsilon_{\theta\theta} & \varepsilon_{r\theta} \\
\varepsilon_{rr} & \varepsilon_{r\theta} & \varepsilon_{zz}
\end{array} \right] \left[ \begin{array}{ccc}
I_{\xi} & 0 & 0 \\
0 & I_{\xi} & 0 \\
0 & 0 & I_{\xi}
\end{array} \right] d\xi_m
\]

\[ + \int_0^{\xi_m} K(\xi_m - \xi') \frac{\partial}{\partial \xi_m} \left[ \begin{array}{ccc}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{array} \right] \left[ \begin{array}{ccc}
3\varepsilon_T & 0 & 0 \\
0 & 3\varepsilon_T & 0 \\
0 & 0 & 3\varepsilon_T
\end{array} \right] d\xi_m \]  
(4-23)
where $\xi_m$ is the reduced time, $G$ and $K$ are the shear and bulk modulus, respectively, $I_e$ is the volume expansion defined previously in Eq. (4-4).

Substituting Eq. (4-4) into Eq. (4-23), the terms having the strain variables can be rewritten as:

\[
\left( \varepsilon_{rr} - \frac{I_e}{3} \right) = \frac{1}{3} \left( 2 \varepsilon_{rr} - \varepsilon_{\theta\theta} - \varepsilon_{zz} \right) \tag{4-24}
\]

\[
\left( \varepsilon_{\theta\theta} - \frac{I_e}{3} \right) = \frac{1}{3} \left( 2 \varepsilon_{\theta\theta} - \varepsilon_{rr} - \varepsilon_{zz} \right) \tag{4-25}
\]

\[
\left( \varepsilon_{zz} - \frac{I_e}{3} \right) = \frac{1}{3} \left( 2 \varepsilon_{zz} - \varepsilon_{rr} - \varepsilon_{\theta\theta} \right) \tag{4-26}
\]

\[
I_e - 3\varepsilon_T = \varepsilon_{rr} + \varepsilon_{\theta\theta} + \varepsilon_{zz} - 3\varepsilon_T \tag{4-27}
\]

where $\varepsilon_T$ is the thermal strain calculated with Eq. (4-6).

Substituting Eqs. (4-24) to (4-27) into Eq. (4-23), it can be rewritten in its stress components as:

\[
\sigma_{rr}(\xi_m(t)) = \int_0^{\xi_m} G(\xi_m - \xi_m) \frac{d}{d\xi_m} \left[ 2\varepsilon_{rr}(\xi_m) - \varepsilon_{\theta\theta}(\xi_m) - \varepsilon_{zz}(\xi_m) \right] d\xi_m
\]

\[
+ \int_0^{\xi_m} K(\xi_m - \xi_m) \frac{d}{d\xi_m} \left[ \varepsilon_{rr}(\xi_m) + \varepsilon_{\theta\theta}(\xi_m) + \varepsilon_{zz}(\xi_m) - 3\varepsilon_T(\xi_m) \right] d\xi_m \tag{4-28}
\]

\[
\sigma_{\theta\theta}(\xi_m(t)) = \int_0^{\xi_m} G(\xi_m - \xi_m) \frac{d}{d\xi_m} \left[ 2\varepsilon_{\theta\theta}(\xi_m) - \varepsilon_{rr}(\xi_m) - \varepsilon_{zz}(\xi_m) \right] d\xi_m
\]

\[
+ \int_0^{\xi_m} K(\xi_m - \xi_m) \frac{d}{d\xi_m} \left[ \varepsilon_{\theta\theta}(\xi_m) + \varepsilon_{rr}(\xi_m) + \varepsilon_{zz}(\xi_m) - 3\varepsilon_T(\xi_m) \right] d\xi_m \tag{4-29}
\]

\[
\sigma_{zz}(\xi_m(t)) = \int_0^{\xi_m} G(\xi_m - \xi_m) \frac{d}{d\xi_m} \left[ 2\varepsilon_{zz}(\xi_m) - \varepsilon_{rr}(\xi_m) - \varepsilon_{\theta\theta}(\xi_m) \right] d\xi_m
\]

\[
+ \int_0^{\xi_m} K(\xi_m - \xi_m) \frac{d}{d\xi_m} \left[ \varepsilon_{zz}(\xi_m) + \varepsilon_{rr}(\xi_m) + \varepsilon_{\theta\theta}(\xi_m) - 3\varepsilon_T(\xi_m) \right] d\xi_m \tag{4-30}
\]
Eqs. (4-28) to (4-30) were discretized using piecewise linear approximation [140].

(The details of the derivation are given in Appendix A). Applying integration by parts and neglecting high order derivatives, the resulting discretized equations are written as:

\[
\sigma_{\theta\theta}^{i,j} = C_1^{\theta\theta} e_{\theta\theta}^{i,j} + C_1^{\theta\theta} (e_{\theta\theta}^{i,j} + e_{\theta\theta}^{i,j-1}) + C_1^{\theta\theta} 
\]

\[
(4-31)
\]

\[
\sigma_{\phi\phi}^{i,j} = C_1^{\phi\phi} e_{\phi\phi}^{i,j} + C_1^{\phi\phi} (e_{\phi\phi}^{i,j} + e_{\phi\phi}^{i,j-1}) + C_1^{\phi\phi} 
\]

\[
(4-32)
\]

\[
\sigma_{rr}^{i,j} = C_1^{rr} e_{rr}^{i,j} + C_1^{rr} (e_{rr}^{i,j} + e_{rr}^{i,j-1}) + C_1^{rr} 
\]

\[
(4-33)
\]

where the superscript \( j \) denote the present time and \( i \) denotes the discretization along the radius.

\( C_1 \) to \( C_5 \) are defined as:

\[
C_1^{\theta\theta} = \left[ \frac{4}{3} \Gamma_{\theta\theta}^{i,j} + K_{\theta\theta}^{i,j} \right] 
\]

\[
(4-34)
\]

\[
C_2^{\theta\theta} = \left[ K_{\theta\theta}^{i,j} - \frac{2}{3} \Gamma_{\theta\theta}^{i,j} \right] 
\]

\[
(4-35)
\]

\[
C_3^{\theta\theta} = \frac{2}{3} \Gamma_{\theta\theta}^{i,j} \left[ -2 e_{\theta\theta}^{i,j-1} + e_{\theta\theta}^{i,j-2} + e_{\theta\theta}^{i,j-3} \right] + \sum_{k=1}^{i-1} \frac{2}{3} \Gamma_{\theta\theta}^{k,j} \left[ 2 e_{\theta\theta}^{k,j} - 2 e_{\theta\theta}^{k+1,j} + e_{\theta\theta}^{k+2,j} - e_{\theta\theta}^{k+3,j} \right] + K_{\theta\theta}^{i,j} \left[ 3 e_{\theta\theta}^{i,j-1} - 3 e_{\theta\theta}^{i,j-2} - e_{\theta\theta}^{i,j-3} \right] 
\]

\[
(4-36)
\]

\[
C_4^{\theta\theta} = \frac{2}{3} \Gamma_{\theta\theta}^{i,j} \left[ -2 e_{\theta\theta}^{i,j-1} + e_{\theta\theta}^{i,j-2} + e_{\theta\theta}^{i,j-3} \right] + \sum_{k=1}^{i-1} \frac{2}{3} \Gamma_{\theta\theta}^{k,j} \left[ 2 e_{\theta\theta}^{k,j} - 2 e_{\theta\theta}^{k+1,j} + e_{\theta\theta}^{k+2,j} - e_{\theta\theta}^{k+3,j} \right] + K_{\theta\theta}^{i,j} \left[ 3 e_{\theta\theta}^{i,j-1} - 3 e_{\theta\theta}^{i,j-2} - e_{\theta\theta}^{i,j-3} \right] 
\]

\[
(4-37)
\]

\[
C_5^{\theta\theta} = \frac{2}{3} \Gamma_{\theta\theta}^{i,j} \left[ -2 e_{\theta\theta}^{i,j-1} + e_{\theta\theta}^{i,j-2} + e_{\theta\theta}^{i,j-3} \right] + \sum_{k=1}^{i-1} \frac{2}{3} \Gamma_{\theta\theta}^{k,j} \left[ 2 e_{\theta\theta}^{k,j} - 2 e_{\theta\theta}^{k+1,j} + e_{\theta\theta}^{k+2,j} - e_{\theta\theta}^{k+3,j} \right] + K_{\theta\theta}^{i,j} \left[ 3 e_{\theta\theta}^{i,j-1} - 3 e_{\theta\theta}^{i,j-2} - e_{\theta\theta}^{i,j-3} \right] 
\]

\[
(4-38)
\]
and

\[ \Gamma^{ij} = \frac{1}{\xi_i} \int_{\xi_{j+1}}^{\xi_j} G(\xi - \xi) \, d\xi \]  \hspace{1cm} (4-39)

\[ K^{ij} = \frac{1}{\xi_i} \int_{\xi_{j+1}}^{\xi_j} K(\xi - \xi) \, d\xi \]  \hspace{1cm} (4-40)

where the superscript \( k \) denotes the discretization of the past time.

The quantities \( C_1 \) to \( C_5 \) are known at the present time, \( j \), when the stresses are calculated. \( C_3 \), \( C_4 \), and \( C_5 \) keep the stress history from the initial time \( t=0 \) to the time \( t=t-\Delta t \). These quantities are functions of the radius since they depend on the relaxation modulus and the strain.

For quasi-static analysis, the equilibrium equations and the strain-displacement relationship contain only spatial derivatives, while the viscoelastic constitutive equation have only operators in the reduced-time variable. Therefore, it is possible that the integration of the equilibrium equation with respect to spatial variables and the integration of the constitutive equations with respect to time can be carried out independently [138]. Based on this, it is assumed that a solution is reached at every time step and the stresses are in equilibrium with the boundary conditions at any instant [137].

Substituting the constitutive equation (Eqs. (4-31) to (4-33)) into the equilibrium equation Eq. (4-18) yields:

\[
\frac{d}{dr}\left( C^{\mu\nu} e^{\mu\nu} + C^{\mu\nu}_2 (e^{\mu\nu}_{\text{ref}} + e^{\mu\nu}_{\text{ref}}) + C^{\mu\nu}_3 \right) +
\frac{1}{r} \left( C^{\mu\nu}_1 e^{\mu\nu} + C^{\mu\nu}_2 (e^{\mu\nu}_{\text{ref}} + e^{\mu\nu}_{\text{ref}}) + C^{\mu\nu}_3 - C^{\mu\nu}_1 e^{\mu\nu}_{\text{ref}} - C^{\mu\nu}_2 (e^{\mu\nu}_{\text{ref}} + e^{\mu\nu}_{\text{ref}}) - C^{\mu\nu}_4 \right) = 0 \]  \hspace{1cm} (4-41)

Substituting the strain-displacement relations (Eqs. (4-19) and (4-20)) into Eq. (4-41) and taking the derivatives with respect to \( r \), we obtain a differential equation in terms
of the radial displacement, \( u_{rr} \) and the axial strain \( \varepsilon_{zz} \). In the plane strain approximation, the strain \( \varepsilon_{zz} \) is constant and independent of radius. Therefore, using the strain \( \varepsilon_{zz} \) instead of the displacement \( u_{zz} \), equivalent expressions are obtained.

\[
C_{ij}^{(j)} \frac{d^2 u_{rr}}{d r^2} + \left[ \frac{d C_{ij}^{(j)}}{d r} + \frac{C_{ij}^{(j)}}{r} \right] \frac{d u_{rr}}{d r} + \left[ \frac{1}{r} \frac{d C_{kj}^{(j)}}{d r} - \frac{C_{kj}^{(j)}}{r^2} \right] u_{rr} \\
+ \left[ \varepsilon_{zz}^{(j)} \frac{d C_{ij}^{(j)}}{d r} + \frac{d C_{ij}^{(j)}}{d r} + \frac{C_{kj}^{(j)}}{r} - \frac{C_{kj}^{(j)}}{r^2} \right] = 0
\] (4-42)

To solve Eq. (4-42), which is a two boundary value problem, the boundary conditions are specified for each problem. In the case of a tube with an inner radius, \( a \), and external radius, \( b \), the inner and outer walls are free of traction forces. Hence, the boundary conditions for the inner and outer walls are written as:

\[
\sigma_r(a,t) = 0 \quad \text{and} \quad \sigma_r(b,t) = 0
\] (4-43)

In the case of rods, the displacement at the center is zero because of symmetry, and the free traction surface this yields:

\[
u_r(0,t) = 0
\] (4-44)

\[
\sigma_r(R,t) = 0
\] (4-45)

Substituting Eqs. (4-19), (4-20) and (4-31) into Eq. (4-45), we obtain the boundary condition at the surface in terms of the displacement, \( u \), written as:

\[
C_{ij}^{(j)} \frac{d u_{rr}^{(j)}}{d r} + C_{ij}^{(j)} \left( \frac{u_{rr}^{(j)}}{R} + \varepsilon_{zz}^{(j)} \right) + C_{ij}^{(j)} = 0
\] (4-46)

The displacement, \( u_{rr} \), is function of the radius only and the strain \( \varepsilon_{zz} \) is constant along the radius for each time step (plane strain approximation). The derivatives in Eq. (4-46) can be discretized using central differences. The final discretization is written as:
\[ u_{n}^{i+i} = u_{n}^{i+i-1} - 2 \frac{C_{r}}{C_{n}} \frac{\Delta r}{R} u_{n}^{i+i} - 2 \Delta r \frac{C_{r}}{C_{n}} C_{n}^{i+j} - 2 \Delta r \frac{C_{r}}{C_{n}} C_{n}^{i-j} \] (4-47)

The node \( u_{n}^{i+i} \) is outside of the solution domain. Then using the equilibrium method [128], Eq. (4-47) is replaced in the solution, as explained in the following section.

4.4 Numerical Implementation

To solve Eq. (4-42) the finite difference method is employed. Discretizing the spatial derivatives using central differences of second order yields:

\[ \frac{d^2 u}{dr^2} = \frac{1}{\Delta r^2} \left[ u_{n+1}^{i+i} - 2 u_{n}^{i+i} + u_{n-1}^{i+i} \right] \] (4-48)

\[ \frac{du}{dr} = \frac{1}{2 \Delta r} \left[ u_{n+1}^{i+i} - u_{n-1}^{i+i} \right] \] (4-49)

Substituting Eqs. (4-48) and (4-49) into Eq. (4-42) yields the following equation for the interior nodes:

\[
\begin{bmatrix}
C_{n}^{i-j} & - \frac{dC_{n}^{i-j}}{dr} \frac{1}{\Delta r} & - \frac{dC_{n}^{i-j}}{dr} \frac{1}{2 \Delta r} & \frac{C_{n}^{i-j}}{2 r \Delta r} & u_{n}^{i+j-1} \\
\frac{dC_{n}^{i-j}}{dr} \frac{1}{\Delta r} & - \frac{dC_{n}^{i-j}}{dr} \frac{1}{\Delta r} & - \frac{dC_{n}^{i-j}}{dr} \frac{1}{2 \Delta r} & \frac{C_{n}^{i-j}}{2 r \Delta r} & u_{n}^{i+j} \\
\frac{dC_{n}^{i-j}}{dr} \frac{1}{\Delta r} & - \frac{dC_{n}^{i-j}}{dr} \frac{1}{\Delta r} & - \frac{dC_{n}^{i-j}}{dr} \frac{1}{2 \Delta r} & \frac{C_{n}^{i-j}}{2 r \Delta r} & u_{n}^{i+j+1} \\
\frac{dC_{n}^{i-j}}{dr} \frac{1}{\Delta r} & - \frac{dC_{n}^{i-j}}{dr} \frac{1}{\Delta r} & - \frac{dC_{n}^{i-j}}{dr} \frac{1}{2 \Delta r} & \frac{C_{n}^{i-j}}{2 r \Delta r} & u_{n}^{i+j+2} \\
\frac{dC_{n}^{i-j}}{dr} \frac{1}{\Delta r} & - \frac{dC_{n}^{i-j}}{dr} \frac{1}{\Delta r} & - \frac{dC_{n}^{i-j}}{dr} \frac{1}{2 \Delta r} & \frac{C_{n}^{i-j}}{2 r \Delta r} & u_{n}^{i+j+3} \\
\end{bmatrix}
\begin{bmatrix}
\Delta - \Delta - \Delta - \\
\Delta + \Delta - \Delta - \\
\Delta + \Delta - \Delta - \\
\Delta + \Delta - \Delta - \\
\Delta + \Delta - \Delta - \\
\end{bmatrix}
\begin{bmatrix}
\varepsilon_{n}^{i} \\
\varepsilon_{n}^{i} \\
\varepsilon_{n}^{i} \\
\varepsilon_{n}^{i} \\
\varepsilon_{n}^{i} \\
\end{bmatrix}
\begin{bmatrix}
\Delta + \Delta - \Delta - \\
\Delta + \Delta - \Delta - \\
\Delta + \Delta - \Delta - \\
\Delta + \Delta - \Delta - \\
\Delta + \Delta - \Delta - \\
\end{bmatrix}
\begin{bmatrix}
\Delta - \Delta - \Delta - \\
\Delta + \Delta - \Delta - \\
\Delta + \Delta - \Delta - \\
\Delta + \Delta - \Delta - \\
\Delta + \Delta - \Delta - \\
\end{bmatrix}
\begin{bmatrix}
u_{n}^{i+j-1} \\
u_{n}^{i+j} \\
u_{n}^{i+j+1} \\
u_{n}^{i+j+2} \\
u_{n}^{i+j+3} \\
\end{bmatrix}
\] (4-50)

Eq. (4-50) is a set of couple algebraic equations that can be arrayed in a band matrix of the form \([A B C][u] = [RHS]\) where \([u]\) is the solution of the displacement at the present time. Eq. (4-50) can be resolved by means of a tridiagonal solver [128].

The boundary condition at the outer wall of the cylinder (tubes and rods) is given by Eq. (4-47). For the case of rods, the boundary condition at the center is given by the symmetry condition, \( u_{r} = 0 \) (zero displacement of the center of the rod). For the case of
tubes, the boundary condition at the inner surface was obtained in a similar way as the boundary condition for the outer wall (Eq. (4-47)).

To obtain the equation for the axial strain $\varepsilon_{zz}$, the axial stress, $\sigma_{zz}$ (Eq. (4-33)) was substituted into the equilibrium condition (Eq. (4-22) yielding:

$$2\pi\int_0^R \left( C_e \varepsilon''_{zz} + C_z \left( \varepsilon''_{\theta\theta} + \varepsilon''_{\theta z}\right) + C_z \right) r dr = 0$$  

(4-51)

The axial strain, $\varepsilon_{zz}$, does not depend on the radius. Therefore, Eq. (4-51) can be solved for $\varepsilon_{zz}$, which yields:

$$\varepsilon_{zz}' = -\frac{\int (C_z (\varepsilon''_{\theta\theta} + \varepsilon''_{\theta z}) + C_z) r dr}{\int (C_z) r dr} = 0$$  

(4-52)

Eqs. (4-50) and (4-52) were solved by iteration. It is important to note that, using Eqs. (4-19 and 4-20), Eq (4-52) is obtained in terms of the displacement $u_{rr}$. Once the strains $\varepsilon_{rr}$, $\varepsilon_{\theta\theta}$ and $\varepsilon_{zz}$ are resolved, the thermally-induced birefringence was calculated from the refractive index tensor (Eq. (4-15)) as follows:

$$n_{rr}^{th} - n_{\theta\theta}^{th} = \int_0^\xi C_e (\xi - \xi) \frac{\partial}{\partial \xi} \left[ \varepsilon_{rr}(\xi) - \varepsilon_{\theta\theta}(\xi) \right] d\xi$$  

(4-53)

$$n_{\theta\theta}^{th} - n_{zz}^{th} = \int_0^\xi C_z (\xi - \xi) \frac{\partial}{\partial \xi} \left[ \varepsilon_{\theta\theta}(\xi) \right] d\xi$$  

(4-54)

$$\Delta n_{zz}^{th} = n_{zz}^{th} - n_{rr}^{th} = \int_0^\xi C_e (\xi - \xi) \frac{\partial}{\partial \xi} \left[ \varepsilon_{rr}(\xi) - \varepsilon_{\theta\theta}(\xi) \right] d\xi$$  

(4-55)

where the superscript $th$ indicates thermal-induced birefringence components.

Using a similar procedure as that used to discretized the stresses described in the Appendix A, the birefringence components can be discretized as follows:

$$\Delta n^a = n^a - n^a = \sum_{i=1}^4 \frac{\varepsilon_{\theta\theta}^{i,k} - \varepsilon_{\theta\theta}^{i,k-1} + \varepsilon_{\theta\theta}^{i,k-1}}{\xi_{i,k} - \xi_{i,k-1}} \int_{\xi_{i,k}}^{\xi_{i,k+1}} C_e (\xi^a_{i,k} - \xi) d\xi$$  

(4-56)
The average birefringence $<n_{zz}^d - n_{zz}^h>$ will be determined integrating numerically Eq. (4-58) using the trapezoidal rule as follows:

$$<n_{zz}^d - n_{zz}^h> = \frac{\Delta r}{2(R - \delta)} \left( (n_{zz}^d - n_{zz}^h)_{R} + (n_{zz}^d - n_{zz}^h)_{\delta} \right) + \frac{\Delta r}{(R - \delta)} \sum_{k=1}^{\frac{\Delta r}{R - \delta}} (n_{zz}^d - n_{zz}^h)^{k}$$

(4-59)

where $\Delta r$ is the step increment the in radial direction.

4.5 Total Residual Stresses and Birefringence

Flow stresses show a maximum near the surface of the molding. In a molded part both flow- and thermally-induced residual stresses are generated throughout the process. As a result, a complex state of stresses result from the competition of flow- and thermally-induced residual stresses distribution throughout the part [141]. Assuming that the coupling effects between thermal- and flow-induced residual stresses are negligible, the total residual stress tensor is:

$$\sigma = \sigma_{res}^{fl} + \sigma_{res}^{th}$$

(4-60)

And the total refraction index is:

$$n = n_0 + n_0^{\delta} + n^h + n^fl = \begin{bmatrix}
  n_{0} + n_{0}^{\delta} + n_{zz}^{\delta} & n_{r}^{\delta} \\
  n_{zz}^{\delta} & n_0 + n_{0}^{\delta} + n_{00}^{\delta} \\
  n_{r}^{\delta} & n_0 + n_{r}^{\delta} + n_{rr}^{\delta}
\end{bmatrix}$$

(4-61)
where the subscripts \( \text{res} \) and superscripts \( \text{fl} \) and \( \text{th} \) stand for residual, flow and thermal, respectively; \( n_0 \) is the initial refractive index and \( \delta_{ij} \) is the unit tensor.

The total birefringence measured in the plane \( r-z \) is:

\[
\Delta n_{\text{Total}} = \Delta n_{\text{res}} = \left[ (\Delta n_{rz}^\beta)^2 + (\Delta n_{rz}^\alpha)^2 + 2(n^\beta_{rz} - n^\alpha_{rz})(\Delta n_{rz}^\alpha) \right]^{\frac{1}{2}}
\]

(4-62)

where the flow-induced birefringence, \( \Delta n_{rz}^\beta \), and thermal-induced birefringence, \( \Delta n_{rz}^\alpha \), are evaluated in Eqs. (3-148) and (4-56), respectively.

The birefringence in the plane \( r-\theta \) is:

\[
\Delta n_{r\theta} = (n^\beta_{rr} - n^\alpha_{rr}) + (n^\beta_{r\theta} - n^\alpha_{r\theta})
\]

(4-63)
CHAPTER V

EXPERIMENTAL

This chapter presents the materials and model parameters used in simulations and the parameters of the Leonov model obtained by fitting the equation of viscosity to the shear-dependent viscosity data. It also describes the equipment and mold geometry employed to obtain the gas-assisted injection moldings under various processing conditions. Furthermore, this chapter explains the methods to measure the distribution of the birefringence components $\Delta n$ and $n_{rr} - n_{\theta\theta}$ along the radius, to measure the average birefringence $<n_{zz} - n_{\theta\theta}>$ along the length of the moldings, and to determine the polymer/gas interface distribution.

5.1 Materials and Model Parameters

In the present work, two general-purpose amorphous polymers were used in experiments and simulations: polystyrene 615 APR 26W supplied by Dow Chemical Co. and polycarbonate Lexan 123 from General Electric. Figs. 5-1 and 5-2 show the experimental and fitted shear-rate-dependent viscosity of PS and PC, respectively. The viscosity of PS was measured at 160, 180, and 200 °C over a wide range of shear rates using a Rheometrics Mechanical Spectrometer, model RMS-800 using the cone and plate mode within low shear rate region and an Instron Capillary Rheometer (Model 3211) at high shear rate region [115]. The viscosity of the polycarbonate was taken from the
Plastics Insight 6.1 Library [142], and it is based on the modified Cross model [143], given by the following equation:

\[
\eta(T, \gamma) = \frac{\eta_0(T)}{1 + \left(\frac{\eta_0(T)\gamma}{\tau^*}\right)^n}
\]

(5-1)

where the zero-shear rate viscosity is defined as:

\[
\eta_0(T) = A \exp\left(\frac{T}{T_b}\right)
\]

(5-2)

where \(\gamma\) is the shear rate, \(\tau^*\) is the shear-stress level at which the viscosity is in the transition between the Newtonian limit and the power-law region, \(A\) is a scaling factor for the viscosity temperature function, \(T_b\) is the measure of temperature sensitivity, and \(n\) is the power-law index. The constants for the Cross model are given in Table 5-1.

In order to determine the rheological parameter \(s\), the viscosity \(\eta_K\), and the relaxation time \(\theta_K\) for each mode of the Leonov equation, the two relaxation modes for PS and three relaxation modes for PC were used in fitting Eq. 5-3 to the viscosity data, shown in Figs. 5-1 and 5-2, at different temperatures by means of least squares method [91].

\[
\eta = \eta_0s + \sum_{k=1}^{n} \frac{2\eta_k}{\left(1 + \frac{4\gamma e \theta_k}{1+e \theta_k}\right)^{1/4}}
\]

(5-3)

The deformation-rate tensor, \(e\), and the zero-shear rate viscosity, \(\eta_0\), were defined previously in Eqs. 3-16 and 3-17, respectively.

The material constants of both polymers used in simulations and the Leonov parameters obtained fitting Eq. 5-3 to the viscosity data are listed in Table 5-2. The
temperature dependence of viscosity and relaxation time were described by the WLF equation.

Figure 5-1 Experimental and fitted viscosity of polystyrene.

Figure 5-2. Theoretical [142] and fitted viscosity of polycarbonate.
Table 5-1 Modified Cross model constants for PC viscosity

<table>
<thead>
<tr>
<th>A (Pa-s)</th>
<th>$T_b$ (K)</th>
<th>$\tau^*$ (Pa)</th>
<th>n</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.03e-7</td>
<td>11227.9</td>
<td>917177.8</td>
<td>0.1</td>
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Table 5-2 Material Constants and Properties of the Polystyrene and Polycarbonate

<table>
<thead>
<tr>
<th>Material constants</th>
<th>PS</th>
<th>PC</th>
<th>Nitrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td>WLF equation:</td>
<td>[11]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>C1</td>
<td>8.285</td>
<td>7.27</td>
<td></td>
</tr>
<tr>
<td>C2 (K)</td>
<td>131.9</td>
<td>164</td>
<td></td>
</tr>
<tr>
<td>Tr (K)</td>
<td>473.5</td>
<td>533</td>
<td></td>
</tr>
<tr>
<td>Leonov model:</td>
<td>[11]</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\eta_1$ (Pa-s)</td>
<td>2230</td>
<td>464</td>
<td></td>
</tr>
<tr>
<td>$\eta_2$ (Pa-s)</td>
<td>447</td>
<td>754.83</td>
<td></td>
</tr>
<tr>
<td>$\eta_3$ (Pa-s)</td>
<td></td>
<td>43.64</td>
<td></td>
</tr>
<tr>
<td>$\theta_1$ (s)</td>
<td>0.1466</td>
<td>0.01</td>
<td></td>
</tr>
<tr>
<td>$\theta_2$ (s)</td>
<td>0.00489</td>
<td>0.00102</td>
<td></td>
</tr>
<tr>
<td>$\theta_2$ (s)</td>
<td></td>
<td>0.00011</td>
<td></td>
</tr>
<tr>
<td>s</td>
<td>4.84e-3</td>
<td>3e-3</td>
<td></td>
</tr>
<tr>
<td>Tait equation:</td>
<td>[11]</td>
<td>[142]</td>
<td></td>
</tr>
<tr>
<td>$\rho_0^g$ ($T_{g}^0$) (Kg/m$^3$)</td>
<td>1021</td>
<td>1160</td>
<td></td>
</tr>
<tr>
<td>$T_{g}^0$ (K)</td>
<td>376</td>
<td>416</td>
<td></td>
</tr>
<tr>
<td>$\alpha_1$ (m$^3$/Kg.K)</td>
<td>5.788x10$^{-7}$</td>
<td>5.71x10$^{-4}$</td>
<td></td>
</tr>
<tr>
<td>$\alpha_2$ (m$^3$/Kg.K)</td>
<td>2.429x10$^{-7}$</td>
<td>2.160x10$^{-7}$</td>
<td></td>
</tr>
<tr>
<td>C</td>
<td>0.0894</td>
<td>0.0894</td>
<td></td>
</tr>
<tr>
<td>$b_{1,1}$ (Pa)</td>
<td>4.615x10$^8$</td>
<td>1.740x10$^8$</td>
<td></td>
</tr>
<tr>
<td>$b_{2,1}$ (K$^{-1}$)</td>
<td>3.019x10$^{-3}$</td>
<td>4.39x10$^{-3}$</td>
<td></td>
</tr>
<tr>
<td>$b_{1,s}$ (Pa)</td>
<td>3.301x10$^8$</td>
<td>2.56x10$^9$</td>
<td></td>
</tr>
<tr>
<td>$b_{2,s}$ (K$^{-1}$)</td>
<td>1.38x10$^{-3}$</td>
<td>2.99x10$^{-3}$</td>
<td></td>
</tr>
<tr>
<td>$b_3$ (K/Pa)</td>
<td>3.2x10$^{-7}$</td>
<td>3.77x10$^{-7}$</td>
<td></td>
</tr>
<tr>
<td>Thermal properties:</td>
<td>[115]</td>
<td>[115]</td>
<td>[115]</td>
</tr>
<tr>
<td>Cp (J/Kg.K)</td>
<td>1420</td>
<td>2150</td>
<td>1040</td>
</tr>
<tr>
<td>K (W/m.s.K)</td>
<td>0.17</td>
<td>0.234</td>
<td>0.0242</td>
</tr>
<tr>
<td>$\rho$ (Kg/m$^3$) at 25 ºC</td>
<td>1040</td>
<td>1052</td>
<td>1.138</td>
</tr>
<tr>
<td>$\rho$ (Kg/m$^3$) at 180 ºC</td>
<td>948</td>
<td>950</td>
<td></td>
</tr>
<tr>
<td>Stress-optical coefficient: $C_\eta$ (Pa$^{-1}$)</td>
<td>[11]</td>
<td>[11]</td>
<td>$-5.2x10^{-9}$</td>
</tr>
</tbody>
</table>
5.2 Equipment and Experimental Procedures

Tubular injection moldings were obtained by GAIM on a Van Dorn 55 HPS-2.8F injection molding machine using a spiral-shaped mold. Fig. 5-3 shows an overall scheme of the GAIM equipment used in experiments. This equipment was developed previously by Shin [144]. It is comprised of an injection-molding machine and the gas-injection system. The injection molding machine is equipped with a shut-off nozzle which delivers the polymer and the gas during the filling and gas-injection stages, respectively. The general specifications of the injection molding machine are reported in Table 5-3. The gas-injection system includes a tank of compressed nitrogen, a Nitrojection™ MTIG10-75-2 pressure-boosting unit, a Tescom™ ER3000 computer-controlled pressure-regulator, and a data-acquisition system using Lab-view programming and National Instrument’s boards [34]. The tank of nitrogen is connected to the pressure-boosting unit which supplies the highly pressurized gas to the pressure regulator. The data acquisition system is connected to the injection molding machine and records the position and velocity of the screw by means of a linear velocity displacement transducer (LVDT). When the specified screw position has been reached, the computer sends the signal to the pressure regulator which triggers the gas at the pressure level previously selected in the computer. The compressed nitrogen coming from the pressure regulator is delivered into the shut-off nozzle through a check valve during the gas injection stage. The data acquisition system also records the gas and mold pressures during the cycle.

The injection molding machine was run in semi-automatic mode during the tests. Before collecting the samples for each run, the machine was allowed to cycle until the processing parameters reached a steady state. To verify the consistency of each run,
samples were weighed on an electronic scale (Sartorius B4100) until three consecutive samples were similar to one another.

![Figure 5-3 Scheme of the GAIM equipment used in experiments.](image)

**Table 5-3 Specifications of the Injection Molding Machine Van-Dorn 55HPS 2.8F**

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clamping force (KN)</td>
<td>500</td>
</tr>
<tr>
<td>Injection Capacity (g)</td>
<td>79.9</td>
</tr>
<tr>
<td>Injection Stroke (mm)</td>
<td>120</td>
</tr>
<tr>
<td>Maximum Injection Pressure (MPa)</td>
<td>172.4</td>
</tr>
<tr>
<td>Screw Diameter (mm)</td>
<td>30</td>
</tr>
<tr>
<td>Barrel L/D Ratio</td>
<td>20</td>
</tr>
<tr>
<td>Maximum Injection Speed (cm/s)</td>
<td>16.8</td>
</tr>
</tbody>
</table>

The mold geometry used to obtain the samples is shown in Fig. 5-4. It consists of two main parts, the sprue and the spiral. The tapered sprue is 72.1 mm long with an entrance diameter of 4.57 mm and an end diameter of 7.4 mm. The sprue is connected perpendicularly to the spiral cavity which has a length of 58 cm and a uniform diameter of 10.1 mm. To record the pressure developed in the mold during the cycle, three Kistler
melt pressure transducers (PT), model 6157B, are mounted in the spiral section of the mold at 52.5 mm, 215 mm, and 342.5 mm from the cavity entrance, as indicated in Fig. 5-4.

Prior to injection molding, the polystyrene and polycarbonate were dried at 80 °C and 105 °C for 4 hours, respectively. As described in Section 2.1, the molding cycle consists of the injection of a specified shot size of polymer into the mold cavity followed by injection of pressurized nitrogen. The gas penetrates the length of the sprue and propagates through the center of the spiral, displacing the molten core and forming the tube-like shaped molding. Fig. 5-5 shows pictorial of the tubular moldings obtained during GAIM experiments. The four different regions of the sample are: 1) the sprue, 2) the primary gas penetration of the spiral, 3) the secondary gas penetration, and 4) the solid region where no gas penetrated at all. The length of the gas penetration and the residual wall thickness vary depending on the molding conditions.
5.3 Birefringence Measurements

A cylindrical coordinate system was used to identify the sample directions with \( z \), \( r \), and \( \theta \) being the flow, radial (velocity gradient), and angular (neutral) direction, respectively. To measure the distribution of the birefringence components \( \Delta n \) and \( n_{rr}-n_{\theta\theta} \) along the radius at different distances from the sprue entrance, slices having a thickness of 0.5 and 1 mm were obtained parallel to the planes \( z-r \) and \( r-\theta \), respectively, as schematically indicated in Fig. 5-6. An Isomet\textsuperscript{TM} low-speed diamond saw was used at 135 RPM to cut the slices. After cutting the samples, the thickness of the slices was measured using a digital micrometer with a resolution of 0.001 mm. The retardation of light on the slices was measured using a Leitz cross-polarized optical microscope with a four-order tilting compensator for PS and a thirty-order compensator for PC. The arrows in Fig. 5-6 indicate the direction of the polarized light used to measure each component of the birefringence. To pinpoint the radial position at which the retardation of the slices
was measured, a scale on the microscope eyepiece and a 40x magnification objective lens were used. The birefringence measurements were started 0.125 mm away from the surface (outer wall) of the molded part since compensation of the light retardation (phase difference) was not possible close to the surface.

The retardation was calculated from the readings of the compensator using the tables and calibration constants provided by the manufacturer. Then, the birefringence was determined from dividing the retardation by the thickness of the sample accordingly to:

\[ \Delta n = \frac{\Gamma}{d} \]  

where \( \Gamma \) is the retardation and \( d \) is the thickness of the sample.

The average birefringence \( <n_{zz} - n_{\theta\theta}> \) was measured using an optical polariscope, Gaertner model L305. This polariscope is equipped with a light source with a wavelength of \( 5.65 \times 10^{-7} \) m and a seven-order Babinet compensator, model L-133-A. The measurements of \( <n_{zz} - n_{\theta\theta}> \) were performed at various positions located at different distances from the sprue entrance along the flow direction, \( z \). Consequently, the polarized light passed through the whole diameter of the sample, as indicated by an arrow in Fig. 5-6.

To measure the residual wall thickness (RWT), the GAIM molding was sectioned using a rotary circular saw at several locations along the flow direction. Subsequently, the cross section was cleaned, and the inner and outer walls de-burred using an exacto knife. After that, the RWT was measured using a caliper with a resolution of 0.02 mm. The gas
penetration length, which includes the length of the sprue, was also measured using a precision caliper.

In the following, \( n_{zz} - n_{\theta \theta} \) will indicate a positive birefringence while \( n_{\theta \theta} - n_{zz} \) will indicate negative birefringence.

Melt injection speed, melt and mold temperature, shot size, gas pressure, and gas-delay time were varied to study the influence of the processing variables on gas penetration and birefringence. The processing conditions used to mold the samples are listed in Table 5-4 and Table 5-5 for PS and PC, respectively. It is important to note that Runs No. 2, 5, 8, 11, 13, and 17 of Table 5-4 were made at the same conditions and they are used as reference.
Table 5-4. Processing Conditions Used to Obtain the Polystyrene Moldings

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>180</td>
<td>85</td>
<td>10.34</td>
<td>7.62</td>
<td>0</td>
<td>60</td>
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<tr>
<td>2</td>
<td>200</td>
<td>85</td>
<td>10.34</td>
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<td>3</td>
<td>230</td>
<td>85</td>
<td>10.34</td>
<td>7.62</td>
<td>0</td>
<td>60</td>
</tr>
<tr>
<td>4</td>
<td>200</td>
<td>75</td>
<td>10.34</td>
<td>7.62</td>
<td>0</td>
<td>60</td>
</tr>
<tr>
<td>5</td>
<td>200</td>
<td>85</td>
<td>10.34</td>
<td>7.62</td>
<td>0</td>
<td>60</td>
</tr>
<tr>
<td>6</td>
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<td>90</td>
<td>10.34</td>
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<td>7</td>
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<td>85</td>
<td>6.89</td>
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<td>10.34</td>
<td>7.62</td>
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<td>85</td>
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<td>7.62</td>
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<td>60</td>
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<td>85</td>
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<td>60</td>
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<td>15.24</td>
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<tr>
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<td>7.62</td>
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<td>30</td>
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<tr>
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<td>200</td>
<td>85</td>
<td>10.34</td>
<td>7.62</td>
<td>0</td>
<td>60</td>
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<td>18</td>
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<td>2.54</td>
<td>0</td>
<td>60</td>
</tr>
</tbody>
</table>

*The shot size of the fully filled mold is 7.315 cm (2.87 in).

Table 5-5. Processing Conditions Used to Obtain the Polycarbonate Moldings

<table>
<thead>
<tr>
<th></th>
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<td>2.54</td>
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CHAPTER VI

SIMULATION AND EXPERIMENTAL RESULTS:
THE EFFECT OF PROCESSING CONDITIONS ON GAS PENETRATION AND
BIREFRINGENCE

This chapter presents the traces of the measured screw position, gas pressure, and mold pressure recorded during the GAIM cycle. The measured mold pressure is contrasted with the simulated mold pressure during both filling and gas penetration stages, to elucidate the dynamics of the GAIM process. Furthermore, this chapter explains the simulated flow-induced transient birefringence developed during the melt and gas injection stages. This study was important to explain the final flow-induced residual birefringence measured in gas-assisted injection moldings. The measured and simulated results of the polymer/gas interface and birefringence distributions in gas-assisted injection moldings obtained under various processing conditions such as: melt and mold temperature, injection speed, shot size, gas pressure, and gas-delay time are presented. The numerical scheme simulates the polymer/gas interface distribution, taking into account the primary and secondary gas penetration that takes place during the molding cycle. This chapter also shows the effect of the slice’s thickness on the measured birefringence $\Delta n$ and $n_{\infty}-n_{00}$ and the measured birefringence components obtained after annealing the samples close to $T_g$.  

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6.1 Dynamics of the GAIM Cycle

Figs. 6-1, 6-3, and 6-5 show the dynamics of the measured cavity pressure developed during the GAIM cycle for PS Runs No. 10, 11, and 12 at injection speeds of 1.27, 7.62, and 15.24 cm/s, respectively. The pressure traces identified as P1, P2, and P3 were recorded by the pressure transducers PT1, PT2, and PT3 installed in the mold cavity as indicated in Fig. 5-4. These figures also show the screw position and the gas pressure with respect to time. Figs. 6-2, 6-4, and 6-6 show the corresponding simulated pressure traces for the GAIM cycle for PS Runs No. 10, 11, and 12. The cycle can be summarized as follows: the shot size, or amount of polymer injected prior to gas injection, is specified by the screw position measured from the fully forward state (zero reference). The cycle starts when the mold closes and the screw moves forward, injecting the polymer into the mold cavity with a constant flow rate. During this process, the mold pressure increases and shows different values at the three pressure transducers according to the pressure gradient along the flow direction. The injection stage finishes when the screw reaches the zero position. At this point, the mold pressure diminishes abruptly when the screw stops, but it does not vanish completely. The initial loss is followed by a gradual pressure reduction that may be caused by the combined effect of volume and normal-stress relaxation due to the compressibility and viscoelasticity of the polymer, respectively. It is also possible that, due to the high injection velocity, the inertial effect of the polymer contributes to this gradual decay of pressure in the mold cavity [145]. Once the screw has reached the zero position, the gas is injected and dwells at constant pressure for five seconds. During this time, the gas penetrates the polymer causing the mold pressure to increase again, reaching a plateau which indicates that the primary gas penetration is
completed and the secondary gas penetration will take place. When the gas-injection time is attained, the pressure regulator relieves the pressure of the injection system. However, the gas inside the sample remains pressurized because the check valve installed in the shut-off nozzle prevents the gas from escaping from the interior of the sample. Consequently, as noted in Figs. 6-1, 6-3, and 6-5, the cavity pressure remained longer than the gas-injection time. In order to vent the gas from the interior of the sample, the injection unit retracts (sprue break) separating the shut-off nozzle from the sprue entrance of the mold. Thus, the pressure at the core of the sample is relieved and the cavity pressure decreases. After the cooling time is attained, the mold is opened and the sample is ejected. Simulation and experiments showed that the filling time (elapsed time between the beginning of the cycle and end of filling) decreased when the injection speed increased.

Figure 6-1 Dynamics of the screw position, gas pressure, and mold pressure during GAIM cycle for PS Run No. 10 at injection speed of 1.27 cm/s.
Figure 6-2 Simulated mold pressure traces during GAIM cycle for PS Run No. 10 at injection speed of 1.27 cm/s.

Figure 6-3 Dynamics of the screw position, gas pressure, and mold pressure during GAIM cycle for PS Run No. 11 at injection speed of 7.62 cm/s.
Figure 6-4 Simulated mold pressure traces during GAIM cycle for PS Run No. 11 at injection speed of 7.62 cm/s.

Figure 6-5 Dynamics of the screw position, gas pressure, and mold pressure during GAIM cycle for PS Run No. 12 at injection speed of 15.24 cm/s.
Also, it can be noted that the time required for the gas to penetrate (elapsed time between the end of filling and the end of the primary gas penetration, indicated by the beginning of the pressure’s plateau during gas injection) decreased when the injection speed increased. This is because high injection speed leads to thinner frozen layer, more temperature increase by viscous heating, and less cooling. All of this, caused a high melt temperature and, as a consequence, low polymer viscosity prior to gas injection.

Simulation and experiments showed that the cavity pressure, during the filling stage, increased with injection speed. However, simulated pressure traces showed a higher magnitude than the measured cavity pressure. This deviation was mainly due to the effect of the frozen layer formed during the filling stage. The frozen layer forms a membrane over the pressure transducer. This caused a deviation between the actual and measured cavity pressure as pointed out by Shin et al. [145] and Isayev et al. [146]. This effect was more evident during the gas penetration stage. It can be observed in Figs. 6-1, 6-3, and 6-
5 (between the end of filling and the gas vent) that the cavity pressure was much lower than the gas pressure. Furthermore, the difference between the measured cavity pressure and gas pressure, during the gas penetration stage, decreased when the injection speed increased. For instance, at the injection speed of 1.27 cm/s (Fig. 6-1), the difference between the measured cavity and gas pressures was more than 40% while at injection speed of 15.24 cm/s (Fig. 6-5), the difference was about 20%. The decrease of the difference between the cavity and gas pressure is due to the reduction of the thickness of the frozen layer. Thinner frozen layer allows the pressure to be transmitted with less loss.

It is important to mention that, in general, the simulated interface distribution showed oscillations. This was especially critical for PC simulations at melt temperatures of 300 and 320 °C. These oscillations can be reduced by refining the mesh, as observed in Fig. 6-7. This figure contrasts the simulated interface distribution for PS Run No. 2 at 79 and 119 meshes along the radius and 216 nodes along the length of the mold. However, by increasing the number of meshes along the radius, the computation time increased from 24 to 40 hours. Therefore, further refinement of the mesh was not considered and the calculations were carried out using 119 meshes along the radius and 216 meshes along the length of the mold. It was also found that, in the output file, the code wrote the initial guess that was not part of the calculations rendering a sharp shoulder at the gas front. This problem was observed in previous simulations performed by Li [50]. In the present calculations the value of the initial guess was removed from the output file. The calculations were performed using the Pentium 4 Cluster at the Ohio Supercomputer Center (OSC).
6.2 Effect of Processing Conditions on Polymer/Gas Interface for PS GAIM Moldings.

One of the most important characteristics of gas-assisted injection moldings is the RWT. This characteristic, in conjunction with the mechanical behavior of the material, plays an important role in defining the stiffness and strength of the molded part. Part stiffness is a measurement of the resistance to deflection under an applied load, and part strength is a measurement of the capability of a part to carry a load. GAIM parts have higher stiffness-to-weight ratios compared to those obtained with CIM. But poorly formed gas channels or thinner RWT than expected reduce the part strength since design loads must be carried by thinner sections [147]. Another important characteristic of these moldings is the gas penetration length which is influenced by the RWT. Process changes which affect the RWT will result in a corresponding change in the gas penetration length for a constant shot size [148]. The following sections present the results of the measurements and simulations of the polymer/gas interface distribution carried out on
gas-assisted tubular injection moldings under various processing conditions. The variables studied were: melt temperature, shot size, injection speed, gas pressure, gas-delay time, and mold temperature.

6.2.1 The Effect of Melt Temperature on Polymer/Gas Interface of PS GAIM Moldings.

Figs. 6-8, 6-9, and 6-10 show the measured and predicted polymer/gas interface distribution with respect to the distance from the sprue entrance for PS Runs No. 1, 2, and 3 at melt temperatures of 180, 200, and 230°C, respectively. The rest of the processing conditions were held constant: shot size of 85%, gas injection pressure of 10.34 MPa (1500 psi), injection speed of 7.62 cm/s (3in/s), gas-delay time of 0 s, and mold temperature of 60°C. It is observed that the simulated RWT was in fair agreement with measurements. Nevertheless, the simulated gas penetration length was longer than measurements at the three temperatures employed.

Figure 6-8 Measured and simulated polymer/gas interface distribution for PS Run No.1 at melt temperature of 180 °C, shot size of 85%, gas injection pressure of 10.34 MPa, injection speed of 7.62 cm/s, gas-delay time of 0 s, and mold temperature of 60 °C.
Figure 6-9 Measured and simulated polymer/gas interface distribution for PS Run No. 2 at melt temperature of 200 ºC, shot of size 85%, gas injection pressure of 10.34 MPa, injection speed of 7.62 cm/s, gas-delay time of 0 s, and mold temperature of 60 ºC.

Figure 6-10 Measured and simulated polymer/gas interface distribution for PS Run No. 3 at melt temperature of 230 ºC, shot size of 85%, gas injection pressure of 10.34 MPa, injection speed of 7.62 cm/s, gas-delay time of 0 s, and mold temperature of 60 ºC.
These figures showed that the tip of the measured polymer/gas interface for the temperature of 180 °C was blunter than that observed at melt temperatures of 200 and 230 °C. As a result, the RWT showed a sharper increase between the primary and secondary gas penetration regions than that observed at high melt temperatures. This effect could have resulted from both a different radius of curvature of the gas front during the gas penetration and a longer secondary gas penetration due to the increase of the melt temperature. The simulations predicted the polymer/gas interface distribution developed during both the primary and secondary gas penetration. A shoulder divides these two regions, showing a sharp transition in the RWT for the three temperatures employed. This might be due to the assumption made about the flat advancing gas front instead of a semispherical- or bullet-like shaped front typically observed when a gas penetrates either viscous [26,27] or viscoelastic fluids [28,29]. To overcome this problem, further simulations must consider a round-shaped gas front taking into account the elongational flow that occurs at the gas advancing front [148]. It is important to mention that the spiral geometry of the mold was not taken into account in the present simulations. Instead, the spiral mold was treated like a straight tube. It was possible that this exclusion also contributes to some of the discrepancies between the simulations and measurements. Another possible source of discrepancies between the simulations and measurements is the design of the gas nozzle. In the present simulations, it was assumed that the gas was injected at the entrance of the sprue, while in the actual experiments, the gas was injected through a check valve located in the shut-off nozzle 4.9 cm before the sprue entrance. Then, the gas first penetrated through the melt contained in the shut-off nozzle channel, which has an inside diameter of 9.5 mm, and then penetrated the sprue and mold cavity.
The polymer displaced by the gas inside the shut-off nozzle may increase the actual shot size with respect to that preset in the injection molding machine leading to a shorter gas penetration length. This phenomenon was not taken into account in the present simulations.

Figs. 6-11 and 6-12 contrast, respectively, the effect of melt temperature on the measured and simulated polymer/gas interface distribution for PS Runs No. 1, 2, and 3. Both simulation and measurements showed that the RWT decreased when the melt temperature increased. Therefore, owing to the constant volume of the mold cavity, the primary gas penetration decreased. However, the thermal shrinkage of the polymer increased with temperature, causing a longer secondary gas penetration. Consequently, it was found in measurements (Fig. 6-11) that the total gas penetration length for Run No. 3 was longer than that of Run No. 2 and comparable with that of Run No. 1. The simulations also showed an increase of the secondary gas penetration when the melt temperature increased. It can be observed in Fig. 6-12 that the simulated total gas penetration length of Run No. 3 was comparable with that of Run No. 2 but shorter than that of Run No. 1. The effect of the melt temperature on the RWT can be explained by the viscoelastic properties of the polymer where the melt temperature plays a fundamental role. Increasing the temperature of the polymer causes a reduction in both the viscosity and elasticity of the polymer. The reduction of the viscosity causes a reduction of the layer of polymer deposited on the wall during the gas penetration stage which in turn is directly related with the formation of the RWT of the molded part [29].
Figure 6-11. Measured polymer/gas interface distribution for PS Runs No. 1, 2, and 3 at melt temperatures of 180, 200, and 230°C, respectively: shot size of 85%, gas injection pressure of 10.34 MPa, injection speed of 7.62 cm/s, gas-delay time of 0 s, and mold temperature of 60 °C.

Figure 6-12 Simulated polymer/gas interface distribution for PS Runs No. 1, 2, and 3 at melt temperatures of 180, 200, and 230°C, respectively: shot size of 85%, gas injection pressure of 10.34 MPa, injection speed of 7.62 cm/s, gas-delay time of 0 s, and mold temperature of 60 °C.
The elasticity of the polymer also plays an important role in the amount of polymer deposited on the wall. This effect was pointed out by Gauri and Koelling [29, 30, 149], who showed that the thickness of the layer of fluid deposited on the wall of a tube during isothermal gas penetration increased with the elasticity of the polymer. Even though the GAIM is a non-isothermal process in which the viscosity is a function of both the temperature and shear-rate during the gas penetration, according to the conclusions drawn in Ref. [149], it can be deduced that the viscoelasticity of the polymer plays an important role on the polymer/gas interface distribution. Also, the viscosity of the polymer has a direct influence on the velocity of the gas penetration, which in turn affects the shear-rate dependent viscosity of the polymer. Thus, the complex interdependence of the polymer melt’s viscoelastic properties with temperature and shear-rate determines the molded part’s RWT and gas penetration length.

The present observations were in agreement with those made by Kapila et al. [32], Jong et al. [36], and Chen et al. [37]. However, Parvez et al. [150] performed GAIM experiments using different gas channels with rib layouts and found that increasing the melt temperature led to longer gas penetration. It is possible that high melt temperatures could cause a longer secondary gas penetration and, as a consequence, the total gas penetration length increased with temperature, as observed between the Runs No. 2 and 3 in Fig. 6-11. Also, increasing the melt temperature could lead to a better packing of the polymer in the thin sections of the mold and, as a consequence, longer gas penetration was observed. This was explained by Shin and Isayev [34]. They found that the gas penetration increased with melt temperature for a standard tensile bar cavity. However,
for high melt temperature they observed a decrease of the gas penetration length and the RWT.

It is important to mention that in the present simulations, the effect of the normal stress difference on the RWT was not included. The viscoelasticity was only taken into account to calculate the pseudoviscosity (Eq. 3-40) to compute the stress build-up and relaxation of stresses and birefringence. Fig. 6-13 contrasts the polymer/gas interface distribution calculated using a viscous [50] and viscoelastic approaches for PS Run No. 2. The difference in the RWT between the viscous and viscoelastic simulations were mainly due to the viscosity fitting of the viscous and viscoelastic models.

![Normalized interface distribution](image)

Figure 6-13 Viscous [50] and viscoelastic simulated polymer/gas interface distribution for PS Run No. 2.

6.2.2 The Effect of Shot Size on Polymer/Gas Interface of PS GAIM Moldings.

One of the most important parameters to control in GAIM is the shot size. Typically in GAIM the polymer occupies between 75-95% of the total volume of the mold cavity [47], so, due to its constant volume, if a large amount of polymer is injected
before the gas injection, short gas penetration is observed because there is less volume available for the gas to penetrate. On the contrary, if the initial amount of polymer in the mold is insufficient, the gas front overtakes the melt front and breakthrough will occur, thus preventing the polymer to fill the cavity completely.

Figs. 6-14, 6-15, and 6-16 show the measured and predicted polymer/gas interface distributions for PS Runs No. 4, 5, and 6 at different shot sizes of 75, 85, and 90%, respectively. The rest of the processing variables were held constant: melt temperature of 200 °C, gas injection pressure of 10.34 MPa (1500 psi), injection speed of 7.62 cm/s (3in/s), gas-delay time of 0 s, and mold temperature of 60 °C. The simulated gas penetration length at a shot size of 75% was shorter than the measured one, while for the shot sizes of 85 and 90% the simulated gas penetration length was longer than the corresponding measured ones. The simulated RWT for the shot sizes of 75 and 85% were in fair agreement with measurements, while the simulated RWT at shot size of 90% resulted considerable thinner than the measured one. Both simulation and experiments showed that gas penetration length decreased when the shot size increased. Therefore, the distance from the gas front to the melt front increased with the shot size. It is important to mention that in the experiment carried out at the shot size of 90%, the gas penetrated the sprue and barely penetrated the spiral region, rendering a large solid region in the sample. One of the possible reasons of the discrepancies in the gas penetration length is the pressure gradient which is proportional to the distance between the gas front and the polymer front. When the shot size was small (i.e. 75%), the gas penetration was longer and the distance from the gas front to the melt front was shorter than that observed at higher shot size.
Figure 6-14 Measured and simulated polymer/gas interface distribution for PS Run No. 4 at shot size 75%: melt temperature of 200 ºC, gas injection pressure of 10.34 MPa, injection speed of 7.62 cm/s, gas-delay time of 0 s, and mold temperature of 60 ºC.

Figure 6-15 Measured and simulated polymer/gas interface distribution for PS Run No. 5 at shot size of 85%: melt temperature of 200 ºC, gas injection pressure of 10.34 MPa, injection speed of 7.62 cm/s, gas-delay time of 0 s, and mold temperature of 60 ºC.
Therefore, the pressure gradient at the solid region was higher leading to a better packing. Conversely, when the shot size increased, the distance from the gas front to the melt front increased significantly, causing a lower pressure gradient in the solid region. Therefore, the packing was not as effective, leading to visible voids especially away from the gas front. Furthermore, the contribution of the melt accumulated in the nozzle (discussed in Section 6.2.1) could have increased the actual shot size leading to a short gas penetration length.

Figs. 6-17 and 6-18 show, respectively, the effect of the shot size on the measured and simulated polymer/gas interface distribution for PS Runs No. 4, 5, and 6. It can be observed that the simulations predicted in qualitative agreement showing that the gas penetration length decreased when the shot size increased.
Figure 6-17 Measured polymer/gas interface distribution for PS Runs No. 4, 5, and 6 at shot sizes of 75%, 85%, and 90%, respectively: melt temperature of 200 °C, gas injection pressure of 10.34 MPa, injection speed of 7.62 cm/s, gas-delay time of 0 s, and mold temperature of 60 °C.

Figure 6-18 Simulated polymer/gas interface distribution for PS Runs No. 4, 5, and 6 at shot sizes of 75%, 85%, and 90%, respectively: melt temperature of 200 °C, gas injection pressure of 10.34 MPa, injection speed of 7.62 cm/s, gas-delay time of 0 s, and mold temperature of 60 °C.
From Fig. 6-17 it is observed that the measured RWT for the shot sizes of 75 and 85% were similar. But the measured RWT for the shot size of 90% was significantly thicker than that of shot sizes of 75 and 85%. Furthermore, the RWT for the shot size of 75% was almost constant from the end of the sprue to the beginning of the secondary gas penetration. Also, it is observed that the tip of the polymer/gas interface at shot size of 75% was blunter than those observed at shot sizes of 85 and 90%, showing a sharper transition of the RWT between the primary and secondary gas penetration regions. This might result from the increase of the distance from the gas front to the end of the cavity (solid region of the molding) when the shot size increased, which led to a longer secondary gas penetration.

Different from other processing conditions, the effect of the shot size on the gas penetration length was evident. Less melt in the cavity resulted in higher volume occupied by the gas. It was evident that the shot size was one of the most critical parameters affecting the gas penetration length. However, it was observed that for shot sizes of 75 and 85%, the RWT were comparable. These observations were in agreement with most of the studies carried out so far [33-35,40]. Potente [40] pointed out that the shot size exerted a strong effect on the gas penetration and small deviations from the set point cause large variations on the gas distribution and reproducibility of the parts. Anders and Sauer [151] defined the “critical melt injection volume” as the minimum volume of polymer injected into the mold that prevents the break-through effect. So, if the critical volume is exceeded, the gas penetration length is reduced and RWT remains unaffected. Nonetheless, it was observed in the present study that for large shot size (i.e. 90%), the measured RWT increased significantly.
6.2.3 The Effect of the Gas Pressure on Polymer/Gas Interface of PS GAIM Moldings

The gas injection pressure has a direct impact on the velocity of the gas during the primary gas penetration. The higher the gas pressure, the faster the gas penetrates the polymer. As a consequence, the velocity field generated during the gas penetration modifies not only the shear-dependent viscosity but also the temperature distribution of the polymer during the gas penetration. The combination of these two effects influences the RWT of the molded part.

Figs. 6-19, 6-20, and 6-21 show the comparison of the predicted and measured gas penetration for PS Runs No. 7, 8, and 9 at gas injection pressures of 6.89 (1000), 10.34 (1500), and 13.79 MPa (2000 psi), respectively. The rest of the processing conditions were held constant: melt temperature of 200 ºC, shot size of 85%, injection speed of 7.62 cm/s (3 in/s), gas-delay time of 0 s, and mold temperature of 60 ºC.

![Graph](image)

Figure 6-19 Measured and simulated gas penetration for PS Run No. 7 at gas pressure of 6.89 MPa: melt temperature of 200 ºC, shot size of 85%, injection speed of 7.62 cm/s, gas-delay time of 0 s, and mold temperature of 60 ºC.
Figure 6-20 Measured and simulated gas penetration for PS Run No. 8 at gas pressure of 10.34 MPa: melt temperature of 200 °C, shot size of 85%, injection speed of 7.62 cm/s, gas-delay time of 0 s, and mold temperature of 60 °C.

Figure 6-21. Measured and simulated gas penetration for PS Run No. 9 at gas pressure of 13.79 MPa; melt temperature of 200 °C, shot size of 85%, injection speed of 7.62 cm/s, gas-delay time of 0 s, and mold temperature of 60 °C.
At low injection pressure 6.89 MPa, the simulated RWT was thicker than the measured one. However, at pressures of 10.34 and 13.79 MPa the simulated and measured RWT were in fair agreement. Furthermore, it was observed that the simulated gas penetration length was longer than the measurements at the three gas pressures.

At high gas pressure, the transition of the RWT between the primary and secondary gas penetration was more gradual than that observed at low gas pressure. It is important to mention that, in the literature, the influence of the gas pressure on the residual wall thickness and gas penetration length vary in importance depending on the type of experiment carried out. The present observations were in agreement with those made by Kapila et al. [32], Shin and Isayev [34], Jong et. al.[36], Chen et al. [46], and Heim [152]. However, Zheng [153] stated that high gas pressure renders lighter parts and longer gas penetration. He attributed this effect to better packing of the part. Nevertheless, he observed that higher gas pressure rendered thinner RWT in the parts.

Other studies performed by Johannaber [148] and Parvez et al. [150] showed that the gas pressure did not have an appreciable influence on the gas penetration length and RWT.

It can be observed that at low gas pressure, the tip of the interface was blunter than that at higher gas pressure. Elevated gas pressure led to fast gas penetration, causing a reduction of the shear-dependent viscosity. Also, fast gas penetration means lower cooling time which led to a higher temperature of melt at the end of the gas penetration stage. This can be observed in Fig. 6-22, where the simulated temperature along the radius at the end of gas penetration at (a) 16 cm and (b) 28 cm from the sprue entrance is presented.
Figure 6-22 Temperature along the radius for Runs No. 7, 8, and 9 at the end of gas penetration at (a) 16 cm and (b) 28 cm from the sprue entrance.

Figs. 6-23 and 6-24 contrast, respectively, the effect of the gas pressure on the measured and simulated polymer/gas interface distributions for PS Runs No. 7, 8, and 9. Measurements and simulations showed that the RWT and the total gas penetration length increased when the gas pressure decreased. Also, measurements and simulations showed that increasing the gas pressure exerted little influence on the secondary gas penetration.

Gas pressure plays an important role in the gas penetration process, as increasing the gas pressure results in higher shear rate and velocity in the polymer domain. The shear rate modifies the viscosity and, as a consequence, the fluidity of the material which in turn affects the polymer/gas interface distribution in GAIM moldings.

Experiments and simulations showed that the gas penetration length and RWT decreased when the gas pressure increased. The shear rate developed during the gas
Figure 6-23. Measured polymer/gas interface distribution for PS Runs No. 7, 8, and 9 at gas pressures of 6.89, 10.34, and 13.79 MPa: melt temperature of 200 °C, injection speed of 7.62 cm/s, gas-delay time of 0 s, and mold temperature of 60 °C.

Figure 6-24. Simulated polymer/gas interface distribution for PS Runs No. 7, 8, and 9 at gas pressure of 6.89, 10.34, and 13.79 MPa: melt temperature of 200 °C, injection speed of 7.62 cm/s, gas-delay time of 0 s, and mold temperature of 60 °C.
penetration stage was considerably lower than the shear rate developed during the injection stage. Therefore, the shear rate’s contribution to the viscous heating, during the gas penetration stage, was minimal. At high gas pressure, the gas displaced the polymer faster towards the end of the cavity and the gas penetrated in less time. As a consequence, when the primary gas penetration finished, the melt temperature was higher than that at lower gas pressure.

The increment of the temperature profile with the gas pressure indicated that the melt temperature during the gas penetration was higher for the highest gas pressure, as shown in Fig. 6-22. Furthermore, when the gas pressure increased, the relatively high shear rate led to a lower viscosity due to shear-thinning effect. Therefore, the polymer melt’s viscosity was lower at the higher gas pressure rendering a thinner RWT and a shorter gas penetration length.

These findings were in agreement with those made by Heim [152], who determined experimentally that the RWT diminishes when the gas-injection pressure increases.

6.2.4 The Effect of the Injection Speed on Polymer/Gas Interface of PS GAIM Moldings.

The melt injection speed is one of the least-discussed processing variables in literature regarding GAIM. This variable plays an important role in defining the rheological state of the polymer melt prior to gas injection. This is because the injection speed directly affects the temperature distribution in both flow and transverse directions [154]. Injection speed also exerts a strong influence in the development of the frozen layer which in turn affects the RWT formation in moldings obtained by GAIM.
Figs. 6-25, 6-26, and 6-27 show the measured and predicted polymer/gas interface distribution for PS Runs No. 10, 11, and 12, at injection speeds of 1.27 (0.5), 7.62 (3), and 15.24 cm/s (6 in/s), respectively. The rest of the processing conditions were held constant: melt temperature of 200°C, shot size of 85%, gas-injection pressure of 10.34 MPa (1500 psi), gas-delay time of 0 s, and mold temperature of 60 ºC. Fig. 6-25 shows that for an injection speed of 1.27 cm/s, simulations overpredicted the RWT while the gas penetration length was underpredicted. At injection speeds of 7.62 and 15.24 cm/s (Figs. 6-26 and 6-27, respectively), the simulated RWT was in fair agreement with the experiments and the simulated gas penetration length was longer than the measured one.

Figure 6-25 Measured and simulated gas penetration for PS Run No. 10 at injection speed of 1.27 cm/s: gas injection pressure of 10.34 MPa, melt temperature of 200 ºC, shot size of 85%, gas-delay time of 0 s, and mold temperature of 60 ºC.
Figure 6-26. Measured and simulated gas penetration for PS Run No. 11 at injection speed of 7.62 cm/s: gas injection pressure of 10.34 MPa, melt temperature of 200 °C, shot size of 85%, gas-delay time of 0 s, and mold temperature of 60 °C.

Figure 6-27. Measured and simulated gas penetration for PS Run No. 12 at injection speed of 15.24 cm/s: gas injection pressure of 10.34 MPa, melt temperature of 200 °C, shot size of 85%, gas-delay time of 0 s, and mold temperature of 60 °C.
One of the reasons for the discrepancy observed in polymer/gas interface
distribution at injection velocity of 1.27 cm/s was that, especially at low injection
velocity, the actual shot size was smaller than the shot size preset in the injection molding
machine. This effect was studied by Shin et al. [35]. Therefore, at low injection velocity,
the actual shot size became less than the set point and, as a consequence, the gas
penetration length increased. At higher injection velocities, the actual shot size was
similar to the preset one [35], and the simulations predicted a longer gas penetration than
the measured one.

Figs. 6-28 and 6-29 show the effect of injection velocity on the measured and
simulated polymer/gas interface distribution at various injection speeds. Measurements
and simulations showed that the gas penetration length and the RWT increased when the
injection speed decreased. The increase of gas penetration length when the injection
speed decreased was due to the fact that low injection speed is proportional to low shear
rate and low viscous heating in the polymer melt during the filling stage. Also, the time
required to complete melt filling was longer, which results in a lower melt temperature
before the gas penetration. This causes an increase of both the solidified layer and the
viscosity near the mold wall, leading to a reduction of the area available for the gas to
penetrate. In Fig. 6-28 it is observed that the measured gas penetration length for the
injection speeds of 7.62 and 15.24 cm/s were similar. However, for the injection speed of
1.27 cm/s, the measured gas penetration length and RWT were significantly higher than
the gas penetration and RWT of the injection speeds of 7.62 and 15.24 cm/s. Simulations
qualitatively agreed with measurements.
**Figure 6-28** Measured polymer/gas interface distribution for PS Runs No. 10, 11, and 12 at injection speeds of 1.27, 7.62, and 15.24 cm/s: melt temperature 200 °C, shot size of 85%, gas injection pressure 10.34 MPa, gas-delay time 0 s, and mold temperature of 60 °C.

**Figure 6-29** Simulated polymer/gas interface distribution for PS Runs No. 10, 11, and 12 at injection speeds of 1.27, 7.62, and 15.24 cm/s: melt temperature of 200 °C, shot size of 85%, gas injection pressure of 10.34 MPa, gas-delay time of 0 s, and mold temperature of 60 °C.
For the injection speed of 15.24 cm/s, the secondary gas penetration increased slightly with respect to that of the two lower injection speeds employed. This could have been caused by the temperature increase due to the viscous heating generated during the filling stage.

It is interesting to observe in Fig. 6-28 that the tip of the measured polymer/gas interface at low injection velocity was blunter than that observed at high injection velocity. Comparing this observation with those made in Section 6.2.1, we can deduce that the temperature of the melt (caused by viscous heating or by higher melt temperature) affects the shape of the advancing gas front and the length of secondary gas penetration resulting in different shapes of the tip of the interface.

These observations were in agreement with the findings of Kapila et al. [32], Zheng [153], and Shin and Isayev [35] who performed an extensive study on the effect of injection speed on the gas penetration length and RWT in GAIM. In these studies they found that the gas penetration length and the RWT increased when the injection speed decreased.

6.2.5 The Effect of the Gas-Delay Time on Polymer/Gas Interface of PS GAIM Moldings.

The gas-delay time is used in GAIM to allow the polymer to cool down in thin sections of the molding, so the incoming gas can only core out the designated thick sections that offer the least resistance [155]. During the gas-delay time, the polymer is static in the mold and the cooling process proceeds faster than during the filling stage. Increasing the gas-delay time causes an increase of the solidified layer and the viscosity.
of the polymer near the mold wall, leading to a reduction of the available area for the gas to penetrate.

Figs. 6-30, 6-31, and 6-32 show the measured and simulated polymer/gas interface distribution for PS Runs No. 13, 14, and 15, at gas-delay times of 0, 3, and 6 s, respectively. The rest of the processing conditions were held constant: melt temperature of 200 °C, shot size of 85%, gas pressure of 10.34 MPa (1500 psi), injection speed of 7.62 cm/s (3 in/s), and mold temperature of 60 °C. These figures show that the simulated gas penetration length at gas-delay time of 0 s (Fig. 6-30), was longer than the measured one, while the simulated RWT was in fair agreement with the measured one. At the gas-delay time of 3 s (Fig. 6-31), the simulated gas penetration length was comparable with the measured one, however, the simulated RWT was thicker than the measured one. At the gas-delay time of 6 s (Fig. 6-32), the present model under-predicted the gas penetration length and the RWT by a large margin. It is possible that the discrepancies observed between the simulations and measurements were caused by an over-prediction of the cooling effect that led to a significant increase of the solidified layer and the polymer viscosity during the delay time. The over-prediction of the cooling could have been due to the constant specific heat capacity and thermal conductivity used in the present simulation as well as the assumption made about the constant temperature at the mold wall [156]. It is important to mention that in both experiment and simulation for PS Run No. 15 the polymer did not fill the cavity completely. In the experiment, the melt front did not reach the end of the cavity, stopping at 62.5 cm from the sprue entrance. In simulations, the melt front stopped at 57.09 cm from the sprue entrance.
Figure 6-30 Measured and simulated polymer/gas interface distribution for PS Run No. 13 at gas-delay time of 0 s, melt temperature of 200 ºC, shot size of 85%, gas injection pressure of 10.34 MPa, injection speed of 7.62 cm/s, and mold temperature of 60 ºC.

Figure 6-31. Measured and simulated polymer/gas interface distribution for PS Run No. 14 at gas-delay time of 3 s, melt temperature of 200 ºC, shot size of 85%, gas injection pressure of 10.34 MPa, injection speed of 7.62 cm/s, and mold temperature of 60 ºC.
Figure 6-32. Measured and simulated polymer/gas interface distribution for PS Run No. 15 at gas-delay time of 6 s, melt temperature of 200 ºC, shot size of 85%, gas injection pressure of 10.34 MPa, injection speed of 7.62 cm/s, and mold temperature of 60 ºC.

Figs. 6-33 and 6-34 show, respectively, the effect of the gas-delay time on the measured and simulated polymer/gas interface distribution. Both measurements and simulations showed that, for the two cases (Runs No. 13 and 14) where the melt front reached the end of the mold cavity, the gas penetration length and the RWT increased with the gas-delay time. The increment of the RWT was due to the increase of the solidified layer during the gas-delay period. This causes a reduction of the area available for the gas to penetrate and lower temperature profile along the radius of the molding due to cooling, as a consequence, the gas penetration length increased. This observation was in agreement with the results obtained by Chen et al. [37] and Potente and Hansen [40]. Parvez et al. [150] observed the same trend near the gate. However, further away from the gate, a reduction of the RWT was observed.
It is important to note that when the gas-delay time increased, the measured RWT at the sprue increased in a higher proportion than that observed at the spiral region. This was because the surface-area to volume ratio in the sprue, whose diameter was significantly smaller than that of the spiral, was greater than that of the spiral region and led to a shorter cooling time. This indicated that the design of the sprue and the location of the gas injection point in the GAIM mold are critical. This is because even though the gas can penetrate the polymer located in the spiral region, the gas penetration will not be possible if the polymer in the sprue solidifies. In the simulation for the gas-delay time of 6 s, the polymer in the sprue becomes so viscous that the fluidity reduced so much that the gas could not penetrate further.

Figure 6-33 Measured gas penetration for PS Runs No. 13, 14, and 15 at gas-delay time of 0, 3, and 6 s, gas injection pressure of 10.34 MPa, melt temperature of 200 °C, shot size 85%, injection speed 7.62 cm/s, and mold temperature of 60 °C.
Figure 6-34 Simulated gas penetration for PS Runs No. 13, 14, and 15 at gas-delay time of 0, 3, and 6 s, gas injection pressure of 10.34 MPa, melt temperature of 200 ºC, shot size of 85%, injection speed of 7.62 cm/s, and mold temperature of 60 ºC.

6.2.6 Effect of the Mold Temperature on Polymer/Gas Interface of PS GAIM Moldings.

Mold temperature determines the rate of heat removal of the polymer during the GAIM cycle. Low mold temperature can cause blemishes on the surface of the molded parts and high mold temperature leads to long cycle times. Thus, adequate selection of mold temperature is important to optimize the cycle and for producing quality parts [155].

Figs. 6-35 and 6-36 show the measured and simulated polymer/gas interface distribution for PS Runs No. 16 and 17, at mold temperatures of 30 and 60 ºC. The rest of the processing conditions were held constant: melt temperature of 200 ºC, shot size of 85%, gas pressure of 10.34 MPa (1500 psi), injection speed of 7.62 cm/s (3 in/s), and gas-delay time of 0 s. From these figures, it is observed that the simulated RWT
Figure 6-35 Measured and simulated polymer/gas interface distribution for PS Run No. 16 at mold temperature of 30 °C: melt temperature of 200 °C, shot size of 85%, gas injection pressure of 10.34 MPa, injection speed of 7.62 cm/s, and gas-delay time of 0 s.

Figure 6-36 Measured and simulated polymer/gas interface distribution for PS Run No. 17 at mold temperature of 60 °C: melt temperature of 200 °C, shot size of 85%, gas injection pressure of 10.34 MPa, injection speed of 7.62 cm/s, and gas-delay time of 0 s.
was in fair agreement with measurements. Also, the total gas penetration length at the mold temperature of 30 ºC was comparable with the measured one. However, the simulated gas penetration length at a mold temperature of 60 ºC was longer than the measured one.

Figs. 6-37 and 6-38 show the effect of mold temperature on the measured and simulated polymer/gas interface distribution for PS Runs No. 16 and 17. Both simulations and measurements showed that the gas penetration length and the RWT increased when the mold temperature decreased. This is because the solidified layer developed during the filling stage increased when the mold temperature decreased. Furthermore, the heat removal was faster at the lower mold temperature leading to an increase of the polymer viscosity near the mold wall. Higher polymer viscosity increases the resistance for the

Figure 6-37 Measured gas penetration for PS Runs No. 16 and 17 at mold temperature of 30 and 60 ºC: gas injection pressure of 10.34 MPa, melt temperature of 200 ºC, shot size of 85%, injection speed of 7.62 cm/s, and gas-delay time of 0 s.
Figure 6-38 Simulated gas penetration for PS Runs No. 16 and 17 at mold temperature of 30 and 60 ºC: gas injection pressure of 10.34 MPa, melt temperature of 200 ºC, shot size of 85%, injection speed of 7.62 cm/s, and gas-delay time of 0 s.

gas to penetrate. This changes the velocity and shear rate profiles during the gas penetration which in turn leads to an increase of the layer of polymer deposited on the wall during the gas penetration.

The present results agreed with the observations made by Kapila et al. [32] and Chen et al. [37]. They observed that increasing the mold temperature increased the RWT and gas penetration length. Potente and Hansen [40] also observed the same trend using a flat mold with a T-shape cross-sectional area. However, Zheng [153] stated that the influence of the mold temperature on the polymer/gas interface distribution was negligible.
6.3 Effect of Injection Speed on Polymer/Gas Interface of PC GAIM Moldings.

Figs. 6-39, 6-40, and 6-41 show the measured and predicted polymer/gas interface distribution with respect to the distance from the sprue entrance for PC Runs No. 1, 2, and 3 at injection speeds of 2.54 (1), 7.62 (3), and 15.24 (6) cm/s (in/s), respectively. The rest of the processing conditions were held constant: melt temperature of 280 °C, shot size of 86.8%, gas pressure of 10.34 MPa (1500 psi), gas-delay time of 0 s, and mold temperature of 30°C. Fig. 6-39 shows that for an injection speed of 2.54 cm/s, the simulated RWT was thicker than the measured one. Also, the simulated gas penetration length was shorter than the measured one. At injection speeds 7.62 and 15.24 cm/s (Figs. 6-40 and 6-41, respectively), the deviation between the simulated and measured gas penetration length and RWT decreased.

Figure 6-39 Measured and simulated polymer/gas interface distribution for PC Run No. 1 at injection speed of 2.54 cm/s: gas injection pressure of 10.34 MPa, melt temperature of 280 °C, shot size 86.8%, gas-delay time of 0 s, and mold temperature of 30 °C.
Figure 6-40 Measured and simulated polymer/gas interface distribution for PC Run No. 2 at injection speed of 7.62 cm/s: gas injection pressure of 10.34 MPa, melt temperature of 280 °C, shot size 86.8%, gas-delay time of 0 s, and mold temperature of 30 °C.

Figure 6-41 Measured and simulated polymer/gas interface distribution for PC Run No. 3 at injection speed of 15.24 cm/s: gas injection pressure of 10.34 MPa, melt temperature of 280 °C, shot size 86.8%, gas-delay time of 0 s, and mold temperature of 30 °C.
The large deviation observed between the measured and simulated RWT at injection velocity of 2.54 cm/s could have been due to an over-prediction of cooling of the melt at low injection speed. Furthermore, at low injection speed, the shot size preset in the injection molding machine may not coincide with the actual shot size as pointed out by Shin [35] and Li [50]. Simulations showed that the length of the secondary gas penetration increased with the injection speed. This was because high injection speed led to a high temperature increase by viscous dissipation, low filling time, and less cooling. Therefore, the polymer shrinkage increased leading to a larger secondary gas penetration.

Figs. 6-42 and 6-43 show, respectively, the effect of injection velocity on the measured and simulated polymer/gas interface distribution for PC Runs No. 1, 2, and 3, at injection speeds of 2.54 (1), 7.62 (3), and 15.24 (6) cm/s (in/s). Measurements and simulation showed that the gas penetration length and the RWT decreased when the injection speed increased. This is because, the time required to complete melt filling was longer for the lowest injection speed. This resulted in a lower melt temperature prior to the gas penetration causing an increase of both the solidified layer and the viscosity near the mold wall. This led to a reduction of the area available for the gas to penetrate rendering a thicker RWT and longer gas penetration.

Figs. 6-44, 6-45, and 6-46 show the measured and predicted polymer/gas interface distribution with respect to the distance from the sprue entrance for PC Runs No. 4, 5, and 6 at injection speeds of 2.54 (1), 7.62 (3), and 15.24 (6) cm/s (in/s), respectively. The rest of the processing conditions were held constant: melt temperature of 300 °C, shot size of 86.8%, gas injection pressure of 10.34 MPa (1500 psi), gas-delay time of 0 s, and mold temperature of 30°C.
Figure 6-42 Measured polymer/gas interface distribution for PC Runs No. 1, 2, and 3 at injection speeds of 2.54, 7.62, and 15.24 cm/s: melt temperature of 280 ºC, shot size of 86.8%, gas injection pressure 10.34 MPa, gas-delay time 0 s, and mold temperature of 30 ºC.

Figure 6-43 Simulated polymer/gas interface distribution for PC Runs No. 1, 2, and 3 at injection speeds of 2.54, 7.62, and 15.24 cm/s: melt temperature of 280 ºC, shot size of 86.8%, gas injection pressure 10.34 MPa, gas-delay time 0 s, and mold temperature of 30 ºC.
Figure 6-44 Measured and simulated polymer/gas interface distribution for PC Run No. 4 at injection speed of 2.54 cm/s: gas injection pressure of 10.34 MPa, melt temperature of 300 °C, shot size 86.8%, gas-delay time of 0 s, and mold temperature of 30 °C.

Figure 6-45 Measured and simulated polymer/gas interface distribution for PC Run No. 5 at injection speed of 7.62 cm/s: gas injection pressure of 10.34 MPa, melt temperature of 300 °C, shot size 86.8%, gas-delay time of 0 s, and mold temperature of 30 °C.
Figure 6-46 Measured and simulated polymer/gas interface distribution for PC Run No. 6 at injection speed of 15.24 cm/s: gas injection pressure of 10.34 MPa, melt temperature of 300 ºC, shot size 86.8%, gas-delay time of 0 s, and mold temperature of 30 ºC.

From Fig 6-46 it is observed that, similarly to PC Run No. 1 (Fig. 6-39), at injection speed of 2.54 cm/s the simulated RWT was thicker and the gas penetration shorter than the corresponding measurements. At injection speeds of 7.62 and 15.24 cm/s (Figs. 6-45 and 6-46, respectively), the difference between the measurements and simulation decreased.

Figs. 6-47 and 6-48 contrast, respectively, the effect of injection velocity on the measured and simulated polymer/gas interface distribution for PC Runs No. 4, 5, and 6 at injection speeds of 2.54, 7.62, and 15.24 cm/s for a melt temperature of 300 ºC. At this melt temperature, similar to melt temperature of 280 ºC (Fig. 6-42 and 6-43), measurements and simulations showed that the gas penetration length and the RWT decreased when the injection speed increased. The tip of the measured polymer/gas interface distribution for the injection speed of 2.54 cm/s was blunter than that at
Figure 6-47 Measured polymer/gas interface distribution for PC Runs No. 4, 5, and 6 at injection speeds of 2.54, 7.62, and 15.24 cm/s: melt temperature of 300 ºC, shot size of 86.8%, gas injection pressure 10.34 MPa, gas-delay time 0 s, and mold temperature of 30 ºC.

Figure 6-48 Simulated polymer/gas interface distribution for PC Runs No. 4, 5, and 6 at injection speeds of 2.54, 7.62, and 15.24 cm/s: melt temperature of 300 ºC, shot size of 86.8%, gas injection pressure 10.34 MPa, gas-delay time 0 s, and mold temperature of 30 ºC.
injection speed of 7.62 and 15.24 cm/s. Furthermore, measurements and simulation showed that the length of the secondary gas penetration increased with the injection speed. This was attributed, as discussed in Section 6.2.4, to both the increase of temperature by viscous heating and a smaller temperature decrease due to cooling.

Figs. 6-49, 6-50, and 6-51 show the measured and predicted polymer/gas interface distribution with respect to the distance from the sprue entrance for PC Runs No. 7, 8, and 9 at injection speeds of 2.54 (1), 7.62 (3), and 15.24 (6) cm/s (in/s), respectively. The rest of the processing conditions were held constant: melt temperature of 320 °C, shot size of 86.8%, gas injection pressure of 10.34 MPa (1500 psi), gas-delay time of 0 s, and mold temperature of 30 °C. Simulations showed that, at injection speed of 2.54 cm/s, the RWT was in fair agreement with measurements. However, the penetration length was shorter than the measured one for the three injection speeds analyzed.

Figure 6-49 Measured and simulated polymer/gas interface distribution for PC Run No. 7 at injection speed of 2.54 cm/s: gas injection pressure of 10.34 MPa, melt temperature of 320 °C, shot size 86.8%, gas-delay time of 0 s, and mold temperature of 30 °C.
Figure 6-50 Measured and simulated polymer/gas interface distribution for PC Run No. 8 at injection speed of 7.62 cm/s: gas injection pressure of 10.34 MPa, melt temperature of 320 °C, shot size 86.8%, gas-delay time of 0 s, and mold temperature of 30 °C.

Figure 6-51 Measured and simulated polymer/gas interface distribution for PC Run No. 9 at injection speed of 15.24 cm/s: gas injection pressure of 10.34 MPa, melt temperature of 320 °C, shot size 86.8%, gas-delay time of 0 s, and mold temperature of 30 °C.
The large difference of gas penetration at a melt temperature of 320 ºC could have been due to large secondary gas penetration due to the extremely high melt temperature. Also, high melt temperature led to a low polymer viscosity which could increase the back-flow in the check valve of the injection molding machine. This effect leads to a difference between the actual shot size and the one preset in the injection molding machine.

Figs. 6-52 and 6-53 contrast, respectively, the effect of injection speed on the measured and simulated polymer/gas interface distribution for PC Runs No. 7, 8, and 9 at injection speeds of 2.54, 7.62, and 15.24 cm/s at melt temperature of 320 ºC. Measurements and simulation showed that the gas penetration length and the RWT decreased when the injection speed increased. For the melt temperature of 320 ºC, the length of the secondary gas penetration increased with injection speed.

Figure 6-52 Measured polymer/gas interface distribution for PC Runs No. 7, 8, and 9 at injection speeds of 2.54, 7.62, and 15.24 cm/s: melt temperature of 320 ºC, shot size of 86.8%, gas pressure of 10.34 MPa, gas-delay time 0 s, and mold temperature of 30 ºC.
6.4 Simulated Transient Birefringence $\Delta n$

The flow-induced birefringence is determined by the thermo-mechanical history that the polymer experiences during the molding process. The build-up and relaxation of shear and normal stresses that takes place during the polymer flow will originate a transient birefringence profile during the molding operation [157]. The combination of the stress build-up and relaxation with the cooling process that the polymer experiences during GAIM determines the final frozen-in residual birefringence in the molded part. In the following sections, the simulated results of the transient birefringence, $\Delta n$, along the radius was analyzed for different processing conditions.
6.4.1 The Effect of Melt Temperature on Simulated Transient Birefringence $\Delta n$

Figs. 6-54, 6-55, and 6-56 show the simulated transient birefringence $\Delta n$ along the radius for PS Runs No. 1, 2, and 3 at melt temperature of 180, 200, and 230 °C, respectively, during the filling (a, c, and e) and gas penetration (b, d, and f) stages at three different locations: (a) and (b) in the sprue region at 4 cm from the entrance, (c) and (d) in the spiral region at 16 cm, and (e) and (f) in the spiral region at 28 cm from the sprue entrance. These figures demonstrate that, during the filling stage, the magnitude of the simulated transient birefringence $\Delta n$ decreased when the melt temperature increased at the three locations analyzed. This is due to the fact that, when the melt temperature increased, the shear and normal stresses developed during the melt injection stage were lower due to the reduction of viscosity and relaxation time of the polymer. It should be noted that the overall magnitude of $\Delta n$ in the sprue was higher than that of the spiral region at the three melt temperatures.

This is because the diameter of the sprue is smaller than that of the spiral region of the cavity. Therefore, owing to the constant flow rate of polymer during the filling stage, the shear and normal stresses developed in the sprue region were higher than the shear and normal stresses developed in the spiral region.

The maximum value of $\Delta n$ at the wall was proportional to the shear and normal stresses present at the time when the control volume was filled at each time step. The birefringence at the center was zero because the velocity gradient at this position vanishes. Therefore, the normal stress difference and the shear stress at the center vanished as well.
Figure 6-54 Simulated transient $\Delta n$ for PS Run No. 1 at a melt temperature of 180 °C: at filling (a, c, and e) and gas penetration (b, d, and f) stages at various distances from the sprue entrance: (a) and (b) at 4 cm, (c) and (d) at 16 cm, and (e) and (f) at 28 cm.
Figure 6-55 Simulated transient $\Delta n$ for PS Run No. 2 at a melt temperature of 200 ºC: at filling (a, c, and e) and gas penetration (b, d, and f) stages at various distances from the sprue entrance: (a) and (b) at 4 cm, (c) and (d) at 16 cm, and (e) and (f) at 28 cm.
Figure 6-56 Simulated transient $\Delta n$ for PS Run No. 3 at a melt temperature of 230 °C: at filling (a, c, and e) and gas penetration (b, d, and f) stages at various distances from the sprue entrance: (a) and (b) at 4 cm, (c) and (d) at 16 cm, and (e) and (f) at 28 cm.
Fig. 6-57 shows the simulated transient shear stresses, the first and second normal differences, the birefringence $\Delta n$, and the shear rate at the end of the filling stage for PS Run No. 2 in the spiral region at 16 cm from the sprue entrance. The magnitude of the first normal stress difference was higher than that of the second normal stress difference. According to Eq. 3-31, the distribution of shear stresses was linear along the radius. This figure also shows that the fast raise of birefringence coincides with the area of higher shear rate.

Figure 6-57 Simulated Birefringence $\Delta n$, first and second normal stress difference, shear rate and shear stresses for PS GAIM molding at 16 cm from the sprue entrance.

In the sprue region, at melt temperature of 180 °C (Fig 6-54a), $\Delta n$ showed a minimum near the mold wall. This minimum was caused by the fast relaxation of stresses due to the local rise in temperature generated by the viscous heating during the injection stage. At a melt temperature of 200 °C (Fig 6-55a), the minimum was not as noticeable as that observed at 180 °C. For the melt temperature of 230 °C (Fig. 6-56a), the effect of viscous heating on the birefringence distribution was the least noticeable of the three melt
temperatures. This is because a higher melt temperature leads to lower melt viscosity. As a consequence, the relative local rise in temperature by viscous heating was lower than that at melt temperatures of 180 and 200 ºC.

In the sprue and spiral regions at 4 and 16 cm from the sprue entrance, respectively, the birefringence distribution developed during the filling stage increased with time at the three melt temperatures (Figs. 6-54a and c, 6-55a and c, and 6-56a and c). Also, $\Delta n$ showed an maximum further away from the outer wall. These two effects were caused by the increase of shear and normal stresses during the filling stage. As time progressed, the viscosity increased and a frozen layer developed near the mold wall. As a result, the frozen layer reduced the cross-sectional area available for the polymer to flow and, due to the constant flow rate during the filling stage, the shear and normal stresses increased causing $\Delta n$ to increase [67]. Furthermore, during the filling stage, the maximum of $\Delta n$ away from the outer wall shifted towards the center as the temperature dropped and the frozen layer grew with time.

In the solid region at 28 cm from the sprue entrance at the three melt temperatures (Figs. 6-54e, 6-55e, and 6-56e), the change of the birefringence profile of $\Delta n$ with respect to time was less marked than that observed at 4 and 16 cm. This is because the melt front took more time to reach this location. Consequently, the elapsed time from when the melt reached this location to the end of the filling stage was shorter than the corresponding elapsed time at the locations of 4 and 16 cm. As a result, there was less time for the polymer to cool down and for the frozen layer to thicken. It also can be observed that at the location of 28 cm at melt temperatures of 180 and 200 ºC, $\Delta n$ decreased with time, while at 230 ºC, $\Delta n$ increased. The decrease of $\Delta n$ observed at melt temperatures of 180
and 200 °C, was due to the temperature increase by viscous heating after the node at this location was filled. The rise in temperature by viscous heating caused a fast relaxation of stresses, as a consequence, ∆n decreased. Conversely, at a melt temperature of 230 °C, the rise in temperature by viscous heating was less important than that at lower melt temperatures. Therefore, the temperature reduction from cooling increased the viscosity of the polymer which in turn increased the shear and normal stresses causing ∆n to increase. For the sake of clarity, the birefringence, ∆n, at a melt temperature of 200 °C and at 28 cm from the sprue entrance is shown in Fig. 6-58. In this figure it is seen that the value of ∆n at 0.4 s was higher than that at 0.6 s. This is because at 0.4 s, the control volume at 28 cm from the sprue entrance had just been filled and the temperature increase by viscous heating was insignificant. At 0.6 s, the birefringence was less than that at 0.4 s due to the local temperature increase by viscous heating, as shown in Fig. 6-59b. This figure shows the simulated distribution of the temperature along the radius

![Figure 6-58 Simulated transient birefringence ∆n for PS Run No. 2 at a melt temperature of 200 °C: during the filling stage at 28 cm from the sprue entrance.](image)

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during the filling and gas penetration stages for PS Run No. 2 in the spiral region at: (a) 16 and (b) 28 cm from the sprue entrance. It is noted that the temperature profile at 0.6 s has a maximum away from the wall that increases with respect to the temperature profile at 0.4 s. Also, as time progresses, the temperature maximum caused by the viscous heating shifted towards the center due to cooling. It is observed that the temperature of the center region was practically uniform due to the low shear rate and low thermal conductivity of the polymer. Near the outer wall, the temperature showed a maximum that increased due to the viscous heating generated by the shear rate and shifted toward the center as time progressed. At the outer wall, the polymer’s temperature was equal to the mold temperature. When the flow stopped, the temperature decreased because of cooling, the maximum near the mold wall vanishes, and the polymer eventually will reach a uniform temperature (mold temperature).

Figure 6-59 Temperature along the radius for Run No. 2 during the filling and gas penetration stages at (a) 16 cm and (b) 28 cm from the sprue entrance.

The temperature maximum near the outer wall coincides with the maximum of shear rate which is shown in Fig. 6-60. This figure shows the shear rate along the radius.
during the filling and gas penetration stages for PS Run No. 2 at a melt temperature of 200 °C at: (a) 16 and (b) 28 cm from the sprue entrance. In both locations, the shear rate increased with radius showing a maximum near the outer wall. Afterward, it decreased to a minimal value near the frozen layer where the viscosity was high because of the decrease of temperature due to cooling. As the time increased and the frozen layer thickened, the maximum of shear rate increased and shifted towards the center. This is because the growth of the frozen layer reduced the cross-sectional area available for the polymer to flow. As a consequence, due to the constant flow rate, the velocity and the shear rate of the polymer increased. During the gas penetration stage (0.82 s and after), the shear rate was significantly lower than that during the filling stage (before 0.82 s) since the gas pressure was significantly lower than the injection pressure.

![Shear rate along the radius for PS Run No. 2 during the filling and gas penetration stages at (a) 16 cm and (b) 28 cm from the sprue entrance.](image)

At the beginning of the primary gas penetration (0.82 s), the birefringence, $\Delta n$, developed at the end of the filling stage (0.8066 s) partially relaxed at each location for 180
the three melt temperatures (Figs. 6-54b, d, and f, 6-55b, d and f, and 6-56b, d and f). This is because the shear and normal stresses generated during the gas penetration were lower than those generated during the filling stage. ∆n relaxed at different rates along the radius, according to the temperature distribution and shear and normal stresses profile developed during the gas penetration stage. It relaxes faster in the core region where the temperature was higher than near the mold wall where the temperature was low because of cooling. The combined effect of the high temperature at the core, the local increase of temperature due to viscous heating, and the temperature drop near the mold wall originated a birefringence relaxation along the radius creating a minimum of ∆n near the outer wall which coincided with the maximum of temperature observed in Fig 6-59. In the sprue region at a melt temperature of 180 ºC (Fig. 6-54b), ∆n showed a pronounced minimum near the wall due to the relatively high temperature increase that took place during the filling stage from viscous heating. At 200 ºC (Fig. 6-55b) this minimum was less marked than that at 180 ºC because the relative temperature increase by viscous heating was less. At 230 ºC (Fig. 6-56b) the minimum of ∆n was the least noticeable among the three melt temperatures, since the polymer’s viscosity at this temperature was the lowest and the corresponding temperature increase from viscous heating was the lowest.

When the gas cored out the cross-sectional area, the birefringence near the newly formed inner wall relaxed due to the elevated temperature of the polymer. Meanwhile, the birefringence near the outer wall, where the polymer temperature has dropped because of the cooling, was frozen-in. It was evident that the gas-injection time decreased when the melt temperature increased. For instance, comparing Figs. 6-54b, 6-55b, and 6-
66b, it is noted that the sprue was cored out faster at the highest melt temperature. Furthermore, due to the fact that the stress-relaxation rate increases with melt temperature, \( \Delta n \) near the inner wall relaxes faster at the highest melt temperature.

In the spiral region at 16 cm from the sprue entrance, the simulated distribution of \( \Delta n \) and its maximum near the outer wall were significantly lower than that observed at the sprue section for the three temperatures analyzed. Also, the minimum of \( \Delta n \) near the outer wall in the spiral region, caused by a combination of cooling and viscous heating effects, was less pronounced that that in the sprue section. Likewise in the sprue region, the birefringence near the outer wall did not relax due to the temperature reduction during the cooling process. While at the center of the sample, the birefringence relaxed due to the elevated melt temperature.

The simulated transient birefringence developed in the solid region at 28 cm from the sprue entrance, showed a similar behavior and slightly lower magnitude than that developed at the location of 16 cm from the sprue entrance. However, because the gas did not core out the location of 28 cm, the value of \( \Delta n \) showed a high relative value along the radius at the end of the primary gas penetration while in the sections where the gas cored out the polymer (e.g. at 4 and 16 cm from the sprue entrance, Figs. 6-54b and 6-54d, respectively) the birefringence relaxed almost completely near the inner wall. This is due to the fact that the shear rate generated at the polymer/gas interface during the gas penetration stage was very low and the stresses near the inner wall relaxed due to the elevated temperature of this region, thus, causing the birefringence to relax.

It is interesting to note that during the gas penetration, the competition between the build-up and relaxation of stresses caused the birefringence increase at certain
positions along the radius as the gas penetration progressed. For instance, at the melt temperature of 180 ºC, $\Delta n$ at 4 cm from the sprue entrance increased slightly near the wall at 0.88 s with respect to $\Delta n$ at 0.84 s (Fig. 6-54b). At 16 (Fig. 6-54d) and 28 cm (Fig. 6-54f) from the sprue entrance, at 4.91 s, $\Delta n$ increased near wall with respect to $\Delta n$ at 0.88 s. At the melt temperature of 200 ºC at 16 and 28 cm from the sprue entrance (Fig. 6-55d and 6-55f, respectively), $\Delta n$ increased near the wall from 0.88 s until the gas cored out this section. For a melt temperature of 230 ºC, the increase of $\Delta n$ during the gas penetration became more significant as noted in Figs. 6-56d and 6-56f. At this melt temperature, $\Delta n$ increased considerably from the time of 0.88 s until the gas cored out the section. This is because at the beginning of gas penetration, the relaxation of the stresses generated during the melt filling was dominant over the stress growth caused by the polymer displacement during the gas penetration. As the gas front advanced and reached the spiral region, owing to its bigger diameter compared to that of the sprue, the amount of polymer displaced by the gas increased. As a result, the stress field generated ahead of the gas front became significant and the birefringence increased. At the lowest melt temperature, the stress relaxation became dominant due to the low gas velocity while at the highest temperature, the stress-build up was more significant due to the fast gas penetration.

After the primary gas penetration finished, the secondary gas penetration took place during further cooling of the polymer. In this stage, the birefringence $\Delta n$ continued relaxing in those parts where the polymer was still hot. Fig. 6-60 shows the development of birefringence $\Delta n$ during the cooling stage in three different locations: (a) in the sprue at 4 cm, (b) in the spiral region at 16 cm, and (c) in the spiral region at 28 cm from the sprue
entrance. The birefringence $\Delta n$ developed in the sprue region (Fig. 6-61a) at the end of the primary gas penetration relaxed almost completely near the inner wall when the primary gas penetration was completed. This was because the polymer near the inner wall was still hot while the birefringence near the outer wall was frozen-in. In the spiral region at 16 cm from the sprue entrance (Fig. 6-61b), the birefringence at the end of the gas penetration near the outer wall relaxed very little. However, near the inner wall, $\Delta n$ showed a small value that eventually relaxed during the subsequent cooling stage.

Figure 6-61 Simulated transient birefringence after the primary gas penetration for PS Run No. 2: (a) in the sprue region, (b) in the primary gas penetration region, and (c) in the solid region.
At 28 cm from the entrance (Fig. 6-61c), \( \Delta n \) also relaxed slightly near the wall, but at the center, the birefringence developed at the end of the primary gas penetration relaxed faster near the center than near the wall. During the secondary gas penetration (at 4.5 s and after), the birefringence near the center did not relax completely. This was because, the gas continued penetrating slowly, pushing the polymer located at the core towards the end of the spiral to compensate for the polymer contraction as it cooled down. It is important to mention that, even though the velocity of the polymer during the secondary gas penetration was extremely low, the decrease of the melt temperature due to cooling made the relaxation time to increase. Therefore, the birefringence did not relax as fast as in those regions where the polymer was cored out.

6.4.2 The Effect of Shot Size on Simulated Transient Birefringence \( \Delta n \)

Figs. 6-62, 6-63, and 6-64 show the simulated evolution of birefringence \( \Delta n \) along the radius for PS Runs No. 4, 5, and 6 at shot sizes of 75, 85, and 90%, respectively, during the filling (a, c, and d) and gas penetration (b, e, and f) at three different locations: (a) and (b) in the sprue at 4 cm from the entrance, (c) and (d) in the spiral region at 16 cm from the entrance, and (e) and (f) in the solid region. These figures show that \( \Delta n \) developed in the same fashion during the filling stage at the three shot sizes. However, due to the difference in the filling time, which is directly proportional to the shot size at constant injection velocity, the value of \( \Delta n \) at the end of the filling stage increased slightly with shot size. This is because a longer filling time led to a lower temperature distribution. This increased the viscosity, which in turn raised the shear and normal stresses and therefore the birefringence. The birefringence profile developed at the end of
the filling stage partially relaxed at the beginning of the gas penetration. At each location, \( \Delta n \) relaxed about the same proportion at the three shot sizes. Nevertheless, in the sprue region, the transient \( \Delta n \) was slightly higher about \( r/R=0.75 \) when the shot size decreased (Figs. 6-62b at 0.74 s, 6-63b at 0.84 s, and 6-64b at 0.93 s). This was caused by the increase of shear rate due to the higher pressure gradient caused by the reduction of the distance from the gas front to the melt front when the shot size decreased. For each of the shot sizes, at 16 cm from the sprue entrance (Fig 6-62d, 6-63d, and 6-64d), it was observed that \( \Delta n \) relaxed at the early stages of the gas penetration, and then increased as the gas penetration progressed. The birefringence increase was greater at the lower shot size because the amount of the polymer located ahead of the gas front was the smallest. This increased the velocity of the melt front, which in turn increased the shear and normal stresses during the gas penetration. For the shot sizes of 75 and 85%, at the end of the gas penetration, the gas cored out this location and the birefringence at the inner wall relaxed while at the shot size of 90% the gas did not core out this location and \( \Delta n \) showed a high magnitude in the center.

For the shot size of 75%, at the end of gas penetration, the gas cored out the location of 28 cm, consequently, the birefringence relaxed significantly near the inner wall (Fig. 6-62f). Furthermore, the birefringence showed a shoulder near the outer wall caused by the temperature drop during the gas penetration. At the shot sizes of 85 and 90% the gas did not penetrate up to 28 cm, and \( \Delta n \) showed a significant value in the core region (Figs. 6-63f and 6-64f). The magnitude of \( \Delta n \) at the end of the gas penetration
Figure 6-62 Simulated transient $\Delta n$ for PS Run No. 4 at shot size of 75%: at filling (a, c, and e) and gas penetration (b, d, and f) stages at various distances from the sprue entrance: (a) and (b) at 4 cm, (c) and (d) at 16 cm, and (e) and (f) at 28 cm.
Figure 6-63 Simulated transient $\Delta n$ for PS Run No. 5 at shot size of 85%: at filling (a, c, and e) and gas penetration (b, d, and f) stages at various distances from the sprue entrance: (a) and (b) at 4 cm, (c) and (d) at 16 cm, and (e) and (f) at 28 cm.
Figure 6-64 Simulated transient $\Delta n$ for PS Run No. 6 at shot size of 90%: at filling (a, c, and e) and gas penetration (b, d, and f) stages at various distances from the sprue entrance: (a) and (b) at 4 cm, (c) and (d) at 16 cm, and (e) and (f) at 28 cm.
stage was lower at the shot size of 90% with respect to $\Delta n$ at the shot size of 85%. This is because when the shot size increased, the pressure gradient between the gas and melt fronts decreased causing the shear and normal stresses to decrease.

Simulations indicated that the gas injection time increased slightly when the shot size decreased. This is because, as discussed in Section 6.2.2, the gas penetration length was inversely proportional to the shot size. Therefore, the amount of polymer between the gas and melt fronts was less when the shot size decreased. This means that, in the case of isothermal gas penetration, the melt front accelerates when this amount reduces as the gas front advances [38]. But in the case of non-isothermal process, the increase of the melt viscosity due to cooling during the gas penetration counterbalanced the melt acceleration, thus, keeping the gas front velocity low. As a consequence, the gas penetration time slightly increased when the shot size decreased. The shoulder of $\Delta n$ that appeared at the end of gas penetration at shot size of 75% and the wide region of $\Delta n$ at the end of the gas penetration (Fig. 6-62f at 1.758 s) demonstrates that the polymer cools down as the gas penetrates.

At the shot size of 75% at 28 cm from the sprue entrance, the birefringence at the inner wall at the end of the gas penetration (Fig. 6-62f at 1.758 s), was higher than the birefringence at the inner wall at 16 cm from the sprue entrance (Fig. 6-62d at 1.758 s). This is because the elapsed time from when the gas cored out the location of 28 cm to the end of the gas penetration stage was shorter than the elapsed time from when the gas cored out the location of 16 cm to the end of the filling stage. Therefore, the birefringence at the inner wall at 16 cm had more time to relax than that at 28 cm.
The variation of $\Delta n$ with the shot size was small compared with the variation of $\Delta n$ caused by other variables. This is because the change of temperature distribution with shot size was not as considerable as that observed in other processing variables (discussed in the following sections). Furthermore, even though the distance from the gas front to the melt front reduced when the shot size reduced, the shear and normal stresses generated during gas penetration were considerably lower than those generated during the filling stage. Therefore, the relaxation of shear and normal stresses developed during the filling stage was dominant over the stress build-up during the gas penetration at the three shot sizes.

6.4.3 The Effect of Gas Pressure on Simulated Transient Birefringence $\Delta n$

Figs. 6-65, 6-66, and 6-67 show the simulated evolution of birefringence, $\Delta n$, along the radius for PS Runs No. 7, 8, and 9 at gas pressure of 6.89 (1000), 10.34 (1500), and 13.79 MPa (2000 psi), respectively, during the filling (a, c, and d) and gas penetration (b, e, and f) at three different locations: (a) and (b) in the sprue at 4 cm from the entrance, (c) and (d) in the spiral region at 16 cm, and (e) and (f) in the spiral region at 28 cm from the sprue entrance. At each location during the filling stage, the birefringence developed in the same manner at the three runs because the processing variables were the same prior to gas injection. At the beginning of gas penetration (0.82 s), the birefringence developed in the injection stage partially relaxed. $\Delta n$ relaxed faster at the lower gas pressure at the three locations analyzed. This is because low gas pressure caused low gas penetration velocity. As a consequence, during the gas penetration, the shear and normal stresses developed in the polymer located ahead of the gas front.
decreased when the gas pressure decreased. Thus, the net effect between the build-up and relaxation of stresses resulted in lower distribution of $\Delta n$ at the lowest gas pressure. During the gas penetration stage at 16 cm from the sprue entrance at the pressure of 6.89 MPa (Fig. 6-65d), $\Delta n$ relaxes in the span of 0.82 to 0.88 s indicating that the stress relaxation mechanism was dominant over the built-up of stresses generated by the polymer displacement during the gas penetration. Then the birefringence near the mold wall increased slightly, showing a shoulder that was formed due to the fast relaxation of $\Delta n$ when the gas cored out the polymer. At the gas pressures of 10.34 MPa and 13.70 MPa (Figs. 6-66d and 6-67d, respectively) the birefringence relaxed at the beginning of gas penetration in the span of 0.82 to 0.84 s. As the gas penetration progressed, $\Delta n$ increased near the mold wall at 0.88 s. This was caused by the increase of shear and normal stresses generated during the gas penetration which in turn was caused by the fast penetration due to the high gas pressure. This indicates that the build-up of stresses became important during the gas penetration stage when the gas pressure increased.

Evidently, the time required for the gas to penetrate the spiral significantly reduced when the gas pressure increased. As a consequence, the gas cored out a specific location (e.g. 4 cm) at different times when the gas pressure increased. For instance, at the gas pressure of 6.89 MPa (Fig. 6-65b), at the time of 0.88 s, the gas still has not cored out the sprue at the location of 4 cm. Although, at gas pressures of 10.34 and 13.79 MPa (Figs. 6-66b and 6-67b, respectively), at the time of 0.88 s, the gas has already cored out the sprue at 4 cm. As a consequence, at the gas pressure of 13.79 MPa at 4 cm from the
Figure 6-65 Simulated transient $\Delta n$ for PS Run No. 7 at gas pressure of 6.89 MPa: at filling (a, c, and e) and gas penetration (b, d, and f) stages at various distances from the sprue entrance: (a) and (b) at 4 cm, (c) and (d) at 16 cm, and (e) and (f) at 28 cm.
Figure 6-66 Simulated transient $\Delta n$ for PS Run No. 8 at gas pressure of 10.34 MPa: at filling (a, c, and e) and gas penetration (b, d, and f) stages at various distances from the sprue entrance: (a) and (b) at 4 cm, (c) and (d) at 16 cm, and (e) and (f) at 28 cm.
Figure 6-67: Simulated transient $\Delta n$ for PS Run No. 9 at gas pressure of 13.79 MPa: at filling (a, c, and e) and gas penetration (b, d, and f) stages at various distances from the sprue entrance: (a) and (b) at 4 cm, (c) and (d) at 16 cm, and (e) and (f) at 28 cm.
sprue entrance (Fig. 6-67b), the birefringence at 0.88 s was lower than the birefringence at the gas pressure of 10.34 MPa (Fig. 6-66b) at the same location and time. This is because, when the gas pressure was high, the gas penetrated the sprue earlier. Therefore, the elapsed time between the core-out and 0.88 s was longer at higher gas pressure.

At the end of the gas penetration stage at 28 cm from the sprue entrance, the gas did not core out this location for the three gas pressures analyzed. The value of $\Delta n$ along the radius increased with the gas pressure. This is because the higher the gas pressure, the faster the gas penetration and the larger the shear and normal stresses in the polymer ahead of the gas front. As a result, at the end of gas penetration, the magnitude of $\Delta n$ was the largest at the highest gas pressure.

6.4.4 The Effect of Injection Speed on Simulated Transient Birefringence $\Delta n$

Figs. 6-68, 6-69, and 6-70 show the simulated evolution of birefringence $\Delta n$ along the radius for PS Runs No. 10, 11, and 12 at injection speeds of 1.27 (0.5), 7.62 (3), and 15.24 (6) cm/s (in/s), respectively, during the filling (a, c, and d) and gas penetration (b, e, and f) at three different locations: (a) and (b) in the sprue at 4 cm from the entrance, (c) and (d) in the sprue region at 16 cm, and (e) and (f) in spiral region at 28 cm from the sprue entrance. During the filling stage, the overall magnitude of the birefringence $\Delta n$ increased with the injection speed at the three locations analyzed. This is because an increase in the injection speed corresponded to an increase of the shear and normal stresses during the injection stage. Also, high injection speed led to low filling time, less cooling of the polymer, and an increase in the local temperature by viscous heating. As a consequence, the frozen layer’s thickness decreased when the injection speed increased.
At each location at injection speed of 1.27 cm/s (Fig. 6-68a, c, and e), $\Delta n$ showed a maximum that shifted away from the wall as time increased. This maximum corresponded to the maximum normal stress differences developed near the solid layer during the injection stage. At an injection speed of 7.62 cm/s (Fig. 6-69a, c, and e), the maximum of $\Delta n$ was closer to the wall than that observed at the injection speed of 1.27 cm/s, since the filling time reduced and the solidified layer had less time to develop. For the injection speed of 15.24 cm/s (Fig. 6-70a, c, and e), the maximum of $\Delta n$ was even closer to the wall due to the fast injection speed, which in turn caused a thin frozen layer. Furthermore, $\Delta n$ showed a noticeable minimum near the outer wall (Fig. 6-70a). This was caused by the fast relaxation of stresses due to the local increase of temperature because of the high shear rate generated at the highest injection speed (15.24 cm/s). At this injection speed, the increase of temperature by viscous heating near the outer wall impeded the birefringence to increase beyond the maximum value observed at the wall.

In the spiral region at 16 cm from the sprue entrance, the magnitude of $\Delta n$ was lower than that observed in the sprue region at the three injection speeds. This is because the stresses in the spiral region were lower than the stresses in the sprue due to the bigger diameter of the spiral. The temperature drop near the wall was more significant at low injection speed, which creates a large area of frozen-in birefringence compared with that observed at higher injection speeds. For an injection speed of 1.27 cm/s, the effect of viscous heating on the birefringence was less than that observed at high injection speed. For instance, the distribution of $\Delta n$ along the radius for the injection speed of 1.27 cm/s
Figure 6-68 Simulated transient $\Delta n$ for PS Run No. 10 at injection speed of 1.27 cm/s: at filling (a, c, and e) and gas penetration (b, d, and f) stages at various distances from the sprue entrance: (a) and (b) at 4 cm, (c) and (d) at 16 cm, and (e) and (f) at 28 cm.
Figure 6-69 Simulated transient $\Delta n$ for PS Run No. 11 at injection speed of 7.62 cm/s: at filling (a, c, and e) and gas penetration (b, d, and f) stages at various distances from the sprue entrance: (a) and (b) at 4 cm, (c) and (d) at 16 cm, and (e) and (f) at 28 cm.
Figure 6-70 Simulated transient $\Delta n$ for PS Run No. 12 at injection speed of 15.24 cm/s: at filling (a, c, and e) and gas penetration (b, d, and f) stages at various distances from the sprue entrance: (a) and (b) at 4 cm, (c) and (d) at 16 cm, and (e) and (f) at 28 cm.
showed a less marked minimum near the outer wall than that at injection speeds of 7.62 and 15.24 cm/s. This minimum was caused due to the increase of temperature by viscous heating, as discussed in Section 6.4.1.

At an injection speed of 1.27 cm/s, in the solid region at 28 cm from the sprue entrance (Fig. 6-68e), \( \Delta n \) developed in a similar manner to that at the location of 16 cm. But the elapsed time from the arrival of the melt front at 28 cm to the end of the filling stage was shorter than the elapsed time from the arrival of the melt front at 16 cm to the end of the filling stage. The difference in the elapsed time between these two locations led to a difference in cooling time and the development of the frozen layer. For this reason, the overall magnitude of \( \Delta n \) was lower at 28 cm than that at 16 cm. It is interesting to note the effect of the viscous heating on \( \Delta n \) at different injection speeds during the injection stage. At injection speed of 1.27 cm/s, the birefringence distribution along the radius increased with time at the three locations analyzed. However, at injection speeds of 7.62 and 15.24 cm/s, the birefringence decreased due to fast stress relaxation caused by the local temperature increase by the viscous heating.

At the beginning of gas penetration, \( \Delta n \) partially relaxed at the three locations analyzed and at the three injection speeds. In particular, at 4 cm from the sprue entrance, for the injection speed of 1.27 cm/s (Fig. 6-68b) \( \Delta n \) relaxed faster further away from the wall and it relaxes all the time. For the injection speed of 7.62 cm/s (Fig. 6-69b) \( \Delta n \) relaxed showing a minimum near the wall. This minimum was a result of the fast relaxation of shear and normal stresses in this region due to the local temperature increase by viscous heating generated during the injection stage. For the injection speed of 15.24 cm/s (Fig. 6-70b), the minimum of \( \Delta n \) was more pronounced. This is because, during the
filling stage, at the higher injection speed the higher local temperature increase in this region by viscous heating. Comparing the three injection speeds at 4 cm from the sprue entrance, it was observed that, for the injection speed of 15.24 cm/s (Fig. 6-70b), when the gas penetration progressed (0.44 s), the birefringence near the outer wall increased because of the increase of shear and normal stresses during the displacement of the polymer by gas. This was a consequence of the fast gas penetration due to the high temperature of the polymer at this particular injection speed. This effect was not observed at lower injection speeds (Figs. 6-68b and 6-69b).

Simulations showed that the gas injection time reduced when the injection speed increased. This is because the temperature of the polymer prior to gas injection was higher at the highest injection speed. High injection speed led to higher temperature increase by viscous heating and shorter injection time which in turn led to less cooling.

At 16 cm from the sprue entrance for the injection speeds of 7.62 and 15.24 cm/s (Figs. 6-69d and 6-70d, respectively) the minimum of $\Delta n$ near the outer wall was less pronounced than that observed in the sprue. This was because the shear rate in spiral region was lower than that of the sprue leading to lower local temperature increase by viscous heating. Similarly, as in the sprue region, this minimum was more pronounced for the injection speed of 15.24 cm/s than for the injection speed of 7.62 cm/s. At this location, for the three injection speeds, the birefringence near the wall increased as the gas penetration progressed. When the gas cores out this location, the birefringence near the inner wall relaxed.

At the 28 cm from the sprue entrance, at the end of the gas penetration, the birefringence along the radius was the highest for the injection speed of 15.24 cm/s (Fig. 6-70d).
This was a consequence of the faster gas penetration that took place when the injection velocity increased.

6.4.5 Effect of the Gas-Delay Time on the Simulated Transient Birefringence \( \Delta n \)

Figs. 6-71 through 6-77 show the simulated transient birefringence \( \Delta n \) along the radius for PS Runs No. 13, 14, and 15. In particular, Fig. 6-71 shows the simulated evolution of \( \Delta n \) for PS Run No. 13 at gas-delay time of 0 s during the filling (a, c, and d) and gas penetration (b, e, and f) stages at three different locations: (a) and (b) in the sprue at 4 cm from the entrance, (c) and (d) in the spiral region at 16 cm, and (e) and (f) in the spiral region at 28 cm from the sprue entrance.

At gas-delay time of 0 s, the simulations indicated that the polymer melt did not stop between the filling and gas penetration stages since the pressure was applied immediately after the completion of the filling. However, as pointed out in Section 6.4.1, the gas pressure was significantly lower than the injection pressure. Therefore, the shear and normal stresses generated during the gas penetration were considerably lower than those generated during the filling stage. However, the stresses developed during the gas penetration stage prevented \( \Delta n \) from relaxing completely. Hence, the birefringence profile during the gas penetration resulted from the net effect of the relaxation of stresses built-up during the injection stage and the stress build-up during the polymer’s displacement by the gas. During the gas penetration, \( \Delta n \) partially relaxed in the core region but it did not relax completely during the gas penetration until the gas cored out the polymer. At this point, \( \Delta n \) relaxed very fast and it had a very low magnitude at the end of the gas penetration.
Figure 6-71 Simulated transient $\Delta n$ for PS Run No. 13 at gas-delay time of 0 s: at filling (a, c, and e) and gas penetration (b, d, and f) stages at various distances from the sprue entrance: (a) and (b) at 4 cm, (c) and (d) at 16 cm, and (e) and (f) at 28 cm.
Fig. 6-72 shows the simulated evolution of birefringence $\Delta n$ for PS Run No. 14 at gas-delay time of 3 s in the sprue region at 4 cm from the sprue entrance at different stages of the cycle: (a) during the filling, (b) during gas-delay time, (c) during the gas penetration stage before the gas cored out the polymer at this location, and d) during the gas penetration stage after the gas cored out the polymer at this location.

During the filling stage at 4 cm from the sprue entrance (Fig. 6-72a), $\Delta n$ developed in the same manner as $\Delta n$ developed at the gas-delay time of 0 s (Fig. 6-71a), since the processing variables were the same during the filling stage. During the delay time (Fig. 6-72b), the birefringence developed at the end of the filling stage (0.8066 s) relaxed faster than that observed when no gas-delay time was employed (Fig. 6-71b). This is because, during the gas-delay time, the polymer was static and the shear rate vanished. Therefore, stress relaxation was the only mechanism that governed the behavior of the birefringence. During the delay time, $\Delta n$ exhibited a minimum near the mold wall due to local temperature increase by the viscous heating during the filling stage. By the end of the gas-delay time (3.81 s), $\Delta n$ relaxed almost completely in the core region where the temperature was still high, while near the mold wall, $\Delta n$ was frozen-in. At the beginning of gas penetration (Fig. 6-72c at 3.85 s), $\Delta n$ increased in the core region showing a maximum further away from the outer wall. In this figure, it is observed that, the birefringence at this maximum increases faster than the birefringence between this maximum and the mold wall. This was because the temperature near the mold wall decreased during the delay time, and the viscosity of the polymer becomes so high that it does not flow during the gas penetration stage. Therefore, the maximum shear rate and
stresses shifted towards the center, causing the maximum of $\Delta n$. The maximum of $\Delta n$ continued increasing as the gas front propagated, reaching its highest value right before the gas cored out the cross-sectional area. When the gas cored out the polymer melt (Fig. 6-72d), $\Delta n$ relaxed more rapidly near the newly formed inner wall where the polymer was still hot, while the birefringence near the outer wall became frozen-in. This difference in
relaxation rate forms the maximum of $\Delta n$ away from the outer wall observed at the end of gas penetration (Fig. 6-72d at 8.81 s).

Fig. 6-73 shows the simulated transient birefringence $\Delta n$ for PS Run No. 14 at gas-delay time of 3 s in the spiral region at 16 cm from the sprue entrance: (a) during the filling, (b) during gas-delay time, (c) during the gas penetration stage before the gas cored out the polymer at this location, and (d) during the gas penetration stage after the gas cored out the polymer at this location. During the filling stage at 16 cm from the sprue entrance (Fig. 6-73a), $\Delta n$ developed in the same manner as $\Delta n$ at the same location at the gas-delay time of 0 s (Fig. 6-71c) since the processing variables were the same prior to gas injection. During the delay time, similarly as in the sprue region, $\Delta n$ relaxed continuously showing a minimum near the outer wall caused by the local increase of temperature by viscous heating. By the end of the delay time, $\Delta n$ relaxed completely in the core region because of the high melt temperature while near the mold wall, where the temperature decreased because of cooling, $\Delta n$ was frozen-in. When the gas started penetrating, $\Delta n$ increased showing a maximum further away from the outer wall that increased until the gas cored out this location. When the gas cored out this location, $\Delta n$ relaxed fast at the newly formed inner wall because the temperature of the polymer in this region was still elevated, while near the mold wall where the temperature decreased due to cooling, $\Delta n$ became frozen-in. This difference in the birefringence-relaxation rate forms the intermediate maximum of $\Delta n$ observed at the end of gas penetration (Fig. 6-73d at 8.81 s).
Figure 6-73 Simulated transient $\Delta n$ for PS Run No. 14 at 16 cm from the sprue entrance (a) filling stage, (b) gas-delay time, (c) gas penetration before core-out, and (d) after core-out.

Fig. 6-74 shows the simulated transient birefringence $\Delta n$ for PS Run No. 14 at gas-delay time of 3 s in the spiral region at 28 cm from the sprue entrance: (a) during the filling stage, (b) during gas-delay time, and (c) during the gas penetration stage. The birefringence developed during the filling stage relaxed during the gas-delay time. It relaxed in the same fashion as the birefringence at the location of 16 cm from the sprue entrance. At the end of the gas-delay time (3.81 s) $\Delta n$ relaxed completely in the core region. During the gas-delay time, the polymer cooled down, the frozen layer developed
and the viscosity near the outer wall increased. Thus, the cross-sectional area of the path of least resistance available for the gas to penetrate reduced. During the gas penetration stage, the gas drove out the polymer at the core. This caused the shear and normal stresses to increase causing the birefringence to increase as the gas penetration progressed. At the end of the gas penetration (Fig. 6-74c), the birefringence showed a maximum (about r/R=0.8) that corresponded to the shear and normal stresses developed during the gas penetration.

Figure 6-74 Simulated transient birefringence $\Delta n$ for Run No. 14 at 28 cm from the sprue entrance (a) filling stage, (b) gas-delay time, and (c) gas penetration stage.
Figs. 6-75 shows the simulated transient birefringence $\Delta n$ for PS Run No. 15 at gas-delay time of 6 s in the spiral region at 4 cm from the sprue entrance: (a) during the filling stage, (b) during gas-delay time, and (c) during the gas penetration stage before the gas cored out the polymer, and (d) after the gas cored out the polymer at this location.

![Graphs showing birefringence changes](image)

Figure 6-75 Simulated transient birefringence $\Delta n$ for PS Run No. 15 at 4 cm from the sprue entrance (a) filling stage, (b) gas-delay time, (c) gas penetration before core out, and (d) after the core-out.

During the filling stage at 4 cm from the sprue entrance (Fig. 6-75a), the birefringence developed in the same manner as $\Delta n$ at gas-delay time of 0 s, since the
processing variables were the same during the filling stage for the three delay-times employed. During the gas-delay time $\Delta n$ relaxed, it relaxed faster at the center where the temperature was still high and the birefringence near the surface was frozen-in. By the end of the delay time, $\Delta n$ at the center relaxed completely. When the gas started penetrating, the birefringence increased again, showing a maximum that increased as the gas penetration progressed.

It can be observed in Fig. 6-75c that the maximum of $\Delta n$ shifted further towards the center in comparison with the maximum of $\Delta n$ at gas-delay time of 3 s (Fig. 6-72c). This is because by increasing the delay time the temperature profile decreased due to cooling, rendering a thicker frozen-in layer. It was also observed that the birefringence developed in the sprue during the gas penetration, increased when the gas-delay time increased. This is because the temperature near the outer wall decreased, leading to a higher viscosity and higher relaxation time. When the gas cored out the polymer, $\Delta n$ relaxed faster near the inner wall and the $\Delta n$ near the outer wall of the tube was frozen-in.

Figs. 6-76 and 6-77 show the simulated transient birefringence, $\Delta n$, for PS Run No. 15 at 16 cm and 28 cm from the sprue entrance, respectively. During the injection stage, $\Delta n$ developed in the same manner as $\Delta n$ at gas-delay time of 0 s, since the processing variables during the injection stage were the same. During the gas-delay time, $\Delta n$ relaxed in the same way as that of gas-delay time of 3 s, since the stress relaxation was the only mechanism that governed the birefringence behavior. By the end of the gas-delay time, $\Delta n$ relaxed almost completely at the center due to the high melt temperature in this region. At these two locations, the gas did not core out the polymer. Nevertheless, it can be observed that the birefringence increased during the gas penetration, but it had a
lower magnitude than that observed in the solid section of the spiral at the gas-delay time of 3 s (Fig. 6-74c).

Figure 6-76 Simulated transient birefringence $\Delta n$ for PS Run No. 15 at 16 cm from the sprue entrance (a) filling stage, (b) gas-delay time, and (c) gas penetration stage.

The low magnitude of $\Delta n$ in the core region was caused by the low flow rate of the polymer that was displaced by the gas due to the small diameter of the gas channel. It was observed that at the gas-delay time of 6 s, the RWT increased and the polymer
displaced, especially in the sprue region, was lower than that of gas-delay time of 0 and 3 s.

![Graphs showing birefringence](image)

Figure 6-77 Simulated transient birefringence $\Delta n$ for PS Run No. 15 at 28 cm from the sprue entrance (a) filling stage, (b) gas-delay time, and (c) gas penetration stage.

6.4.6 The Effect of Mold Temperature on Simulated Transient Birefringence $\Delta n$

Figs. 6-78 and 6-79 show the simulated transient birefringence $\Delta n$ along the radius for PS Runs No. 16 and 17 at mold temperatures of 30 and 60 °C, respectively,
during the filling (a, c, and d) and gas penetration (b, e, and f) stages at three different locations: (a and b) in the sprue at 4 cm from the entrance, (c and d) and (e and f) in the spiral region at 16 and 28 cm from the sprue entrance, respectively.

During the filling stage, the magnitude of $\Delta n$ along the radius decreased when the mold temperature increased. The difference of $\Delta n$ between the mold temperatures of 30 and 60 ºC was more noticeable near the mold wall than in the center of the cavity, where their magnitudes were similar. This is because, during the injection stage, the competition between the heat removal by the mold wall and the temperature increase by viscous heating keeps the polymer in the core region nearly isothermal. On the contrary, near the mold wall, at the lowest mold temperature, the temperature dropped because of the increase of the heat removal rate. This increased the viscosity of the polymer, leading to an increase of the shear and normal stresses and birefringence.

For each location, the maximum of $\Delta n$ shifted away from the wall when the mold temperature decreased. This is because the lower temperature of the polymer melt (at the lower mold temperature) led to a higher viscosity along the radius. As a consequence, the shear and normal stresses increased, leading to a higher value of $\Delta n$.

During the gas penetration, $\Delta n$ partially relaxed at each location with a similar pattern at both mold temperatures. However, the minimum of $\Delta n$ near the outer wall shifted further towards the center at the lower mold temperature. This was because the maximum of temperature caused by the viscous heating at mold temperature of 30 ºC, shifted further towards the center due to cooling than that at the mold temperature of 60 ºC. Therefore, the fast stress relaxation in this region caused $\Delta n$ to decrease. During the
Figure 6-78 Simulated transient $\Delta n$ for PS Run No. 16 at mold temperature of 30 ºC: at filling (a, c, and e) and gas penetration (b, d, and f) stages at 4 (a and b), 16 (c and d), and 28 (e and f) cm from the sprue entrance.
Figure 6-79 Simulated transient birefringence $\Delta n$ for PS Run No. 17 at mold temperature of 60 °C: at filling (a, c, and e) and gas penetration (b, d, and f) stages at 4 (a and b), 16 (c and d), and 28 (e and f) cm from the sprue entrance.
gas penetration stage, the temperature increase by viscous heating was almost negligible in comparison to that during the filling stage because the shear rate was significantly lower than that of the filling stage.

The gas penetration time decreased slightly when the mold temperature increased. This is because a higher mold temperature corresponded to a lower rate of heat removal and the polymer’s temperature distribution increased. As a consequence, the polymer’s viscosity was low and the gas took less time to penetrate.

6.5 The Effect of the Processing Conditions on Birefringence of PS GAIM Moldings.

The preceding sections presented the effect of the processing conditions on the simulated transient birefringence. The flow-induced residual birefringence is determined by the thermo-mechanical history that the material experienced during the GAIM process. Therefore, the manner that the flow-induced birefringence evolves determines the residual birefringence in GAIM moldings. In the following sections, measured residual birefringence \( \Delta n \) and \( n_{rr}-n_{\theta\theta} \) on slices of different thicknesses is presented, and the simulated flow-induced birefringence components \( \Delta n \) and \( n_{rr}-n_{\theta\theta} \) are compared with measurement in gas-assisted molded parts obtained under different processing conditions.

6.5.1 Effect of the Slice’s Thickness on the Measured Birefringence \( \Delta n \) and \( n_{rr}-n_{\theta\theta} \).

To study the effect of the thickness of the slices removed from the GAIM moldings on the measured birefringence distribution of \( \Delta n \) and \( n_{rr}-n_{\theta\theta} \), slices having different thicknesses were obtained. Fig. 6-80 shows the measured birefringence (a) \( \Delta n \) and (b) \( n_{rr}-n_{\theta\theta} \) for PS Run No. 10 at 17 cm from the sprue entrance at different
thicknesses. It was observed that the measured $\Delta n$ showed small differences. These differences could have been caused due to the cutting. For the birefringence $n_{rr}-n_{\theta\theta}$ the difference between 0.5 and 1 mm was more evident. However, the magnitude of the birefringence near to outer wall was not altered significantly.

For the PC GAIM moldings, the distribution of measured $\Delta n$ was strongly influenced by the thickness of the slices cut from the PC GAIM moldings. Fig. 6-81 shows the measured distribution of $\Delta n$ (a) and $n_{rr}-n_{\theta\theta}$ (b) for PC Run No. 7 at 17 cm from the sprue entrance, at different slice thicknesses: 0.5 mm, 1 mm, and 2 mm. For a slice thickness of 0.5 mm, it was observed that the birefringence was positive through the wall thickness. When the sample thickness was increased, the measured $\Delta n$ and $n_{rr}-n_{\theta\theta}$ showed a maximum near the outer wall, decreased passing through zero to a negative minimum, and then increased passing once more through zero to a positive maximum near the inner...
wall. When the thickness of the slices were increased to 2 mm, the distribution of $\Delta n$ and $n_{rr} - n_{\theta\theta}$ were similar to those at the slice thickness of 1 mm. However, the negative minimum of $\Delta n$ and $n_{rr} - n_{\theta\theta}$ was lower and the birefringence near the inner wall decreased.

Figure 6-81 Measured birefringence $\Delta n$ and $n_{rr} - n_{\theta\theta}$ for PC Run No. 7 at different slice thicknesses (a) 0.5 mm, (b) 2 mm, and (c) 3 mm, between 16 and 17 cm from the sprue entrance.

For slices with a thickness of 0.5 mm, the birefringence $\Delta n$ and $n_{rr} - n_{\theta\theta}$ showed a positive magnitude throughout the wall thickness. When the thickness of the slices was increased to 2 mm, both $\Delta n$ and $n_{rr} - n_{\theta\theta}$ showed a positive maximum near the outer wall of the molding. It decreased passing through zero to a negative minimum. Then, the birefringence increased passing once more through zero to a positive region. When the thickness of the slices was increased to 3 mm, both $\Delta n$ and $n_{rr} - n_{\theta\theta}$ showed a similar behavior than that of the measured birefringence in a slice of 2 mm. However, the minimum was lower. Furthermore, the magnitude of the measured $n_{rr} - n_{\theta\theta}$ increased near the inner wall. The differences observed in the measured birefringence when the
thickness of the slices was varied, might have been due to relaxation of the stresses that
took place when the three-dimensional distribution of the residual stresses was altered
during the removal of the slice. Also, it is important to mention that, due to the circular-
cross sectional area of the GAIM moldings employed in the present work (Fig. 5-5), the
thickness of the slice in the plane \( z-r \) (Fig. 5-6) could not have been increased since the
light, which passes through the tangential direction, \( \theta \), would have crossed points located
at different distances from the center.

6.5.2 The Effect of Melt Temperature on Birefringence of PS GAIM Moldings.

Figs. 6-82, 6-83, and 6-84 show the measured and simulated results of residual
birefringence \( \Delta n \) and \( n_{rr}-n_{\theta\theta} \) for PS Runs No. 1, 2, and 3 at melt temperatures of 180, 200,
and 230 °C, respectively, at various distances from the sprue entrance: (a) and (b) in the
sprue region at 4 and 6.5 cm, (c) and (d) in the primary gas penetration of the spiral at 11
and 16 cm, and (e) in the solid region at 28 cm. It is important to note that the measured
birefringence components \( \Delta n \) and \( n_{rr}-n_{\theta\theta} \) were not fully symmetric with respect to the
center of the spiral. This could be caused by error introduced during measurements and/or
small temperature differences between the two halves of the mold. At each location for
the three melt temperatures, the measured birefringence components \( \Delta n \) and \( n_{rr}-n_{\theta\theta} \)
showed a maximum at the outer wall. Then, both components decreased showing a
plateau further away from the outer wall. The difference between \( \Delta n \) and \( n_{rr}-n_{\theta\theta} \) near the
outer wall was about one order of magnitude, whereas in the plateau region their
magnitudes were similar.
Figure 6-82 Measured and simulated birefringence distribution of $\Delta n$ and $n_{rr}-n_{00}$ at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm. for PS Run No. 1 at melt temperature of 180 ºC.
Figure 6-83 Measured and simulated birefringence distribution of $\Delta n$ and $n_{00} - n_{rr}$ at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm. for PS Run No. 2 at melt temperature of 200 ºC.
Figure 6-84 Measured and simulated birefringence distribution of $\Delta n$ and $n_{\theta\theta} - n_{rr}$ at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm. for PS Run No. 3 at melt temperature of 230 ºC.
In the sprue region, the maximum birefringence $\Delta n$ at the outer wall decreases with respect to the distance from the sprue entrance, while in the primary gas penetration region of the spiral the maximum of $\Delta n$ remained almost constant. The maximum birefringence, $\Delta n$, at the outer wall in the primary gas penetration region of the spiral was significantly lower than the maximum of $\Delta n$ in the sprue region. Nevertheless, at the inner wall, $\Delta n$ exhibited a similar value in both regions. The simulated birefringence components, $\Delta n$ and $n_{rr}-n_{\theta \theta}$, at different distances from the sprue entrance, showed a maximum value near the outer wall. Then, they decreased to zero near the inner wall. The maximum of the simulated $\Delta n$ decreased along the sprue region and remained almost constant in the primary gas penetration region of the spiral. However, in the solid region, the maximum of $\Delta n$ was slightly lower than that of the primary gas penetration region of the spiral.

In general, the maximum of the measured birefringence, $\Delta n$, near the outer wall decreased when the melt temperature increased. As discussed in Section 6.4.1, this is because the polymer’s viscosity decreased when the temperature increased. This led to a lower shear and normal stresses during the filling and gas penetration stages. Furthermore, the relaxation time, which inversely proportional to the melt temperature, decreased causing a faster relaxation of the birefringence. The simulated results showed a qualitative agreement with the measurements. Nevertheless, the simulated birefringence $\Delta n$ showed a higher magnitude than the measured $\Delta n$. One of the reasons of this over-prediction, especially at the melt temperature of 180 ºC, can be the over-prediction of cooling. Also, the stress-optical rule has a limiting value, the birefringence increases with the stresses but at high normal and shear stresses its value deviates from the linear
behavior [93]. Also it can be observed that the birefringence $n_{rr}-n_{\theta\theta}$ near the outer wall was significantly lower than $\Delta n$ but near the inner wall, their magnitudes were comparable. Simulations and measurements showed that birefringence $n_{rr}-n_{\theta\theta}$ was one order of magnitude lower than $\Delta n$. And its value was almost comparable among the different temperatures.

The simulated flow-induced $\Delta n$ for a melt temperature of 180 °C showed a shoulder at all the locations analyzed. For a melt temperature of 200 °C, $\Delta n$ only exhibited a shoulder in the solid region at the location of 28 cm. At the melt temperature of 230 °C, simulated $\Delta n$ did not show any shoulder. As discussed in Section 6.4.1, this shoulder was formed during the gas penetration stage when the gas displaced the polymer at the core creating a shear and normal stresses profile. Simulations showed that the magnitude of shoulder of $\Delta n$ at the location of 28 cm decreased when the melt temperature increased. This is because high melt temperature led to a faster stresses and birefringence relaxation when the polymer flow stopped.

6.5.3 The Effect of Shot Size on Birefringence of PS GAIM Moldings.

Figs. 6-85, 6-86, and 6-87 show the measured and simulated residual flow-induced birefringence $\Delta n$ and $n_{rr}-n_{\theta\theta}$ along the radius for PS Runs No. 4, 5, and 6 at shot sizes of 75, 85, and 90%, respectively, at different distances from the sprue entrance: (a) and (b) in the sprue region at 4 and 6.5 cm, (c) and (d) in the primary gas penetration of the spiral region at 11 and 16 cm, and (e) in the solid region of the spiral at different locations depending on the shot size.
Figure 6-85 Measured and simulated birefringence distribution of $\Delta n$ and $n_{rr}-n_{00}$ at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 45 cm. for PS Run No. 4 at shot size of 75%.
Figure 6-86 Measured and simulated birefringence distribution of $\Delta n$ and $n_{rr} - n_{00}$ at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm. for PS Run No. 5 at shot size of 85%.
These figures show that the maximum of the measured birefringence $\Delta n$ and $n_{rr}-n_{\theta\theta}$ at the outer wall, remained almost constant when the shot size increased. It was found that the shot size did not exert a significant influence on the magnitude of neither $\Delta n$ nor $n_{rr}-n_{\theta\theta}$. At the locations of 4, 6.5 and 11 cm, the simulated flow-induced $\Delta n$ and $n_{rr}-n_{\theta\theta}$ exhibited almost the same value along the radius of the sample for the three shot sizes. However, in the solid region of the molding, the magnitude of the shoulder of $\Delta n$
decreased when the shot size increased. This is because, at low shot size, the speed of the
gas front increased. This increased the birefringence induced by flow, as discussed in
Section 6.4.2.

As discussed in Section 6.2.2, the gas penetration length decreased when the shot size increased. As a consequence, the solid region of the spiral increased. For instance, for the shot size of 90%, the gas front did not reach the location of 16 cm from the sprue entrance. Therefore, the birefringence at this location (Fig 6-87d) behaved in the same way as the birefringence in solid region of the moldings obtained at shot sizes of 75 and 85% (Figs. 6-85e and 6-86e), respectively.

6.5.4 The Effect of Gas Pressure on Birefringence of PS GAIM Moldings.

Figs. 6-88, 6-89, and 6-90 show the measured and simulated residual
birefringence $\Delta n$ and $n_{rr} - n_{\theta\theta}$ along the radius for PS Runs No. 7, 8, and 9, at gas pressures
of 6.89 (1000), 10.34 (1500) and 13.79 MPa (2000 psi), respectively, at different
distances from the sprue entrance: (a) and (b) in the sprue region at 4 and 6.5 cm, (c) and
(d) in the primary gas penetration region of the spiral at 11 and 16 cm, and (e) in the solid
region of the spiral at 28 cm. In general, the measured birefringence $\Delta n$ showed a
maximum near the outer wall, it decreased steeply and showed a plateau toward the inner
wall (in the gas penetration region) and in the core (in the solid region of the spiral). The
maximum of $\Delta n$ near the outer wall and the plateau near the inner wall were similar for
the three gas pressures employed. The measured birefringence $n_{rr} - n_{\theta\theta}$ exhibited the same
order of magnitude near the inner and outer walls of the molding.
Figure 6-88 Measured and simulated birefringence distribution of $\Delta n$ and $n_{00}^\prime n_{rr}$ at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm. for PS Run No. 7 at gas pressure of 6.89 MPa.
Figure 6-89 Measured and simulated birefringence distribution of $\Delta n$ and $n_{0\theta/0\theta}$ at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm. for PS Run No. 8 at gas pressure of 10.34 MPa.
Figure 6-90 Measured and simulated birefringence distribution of $\Delta n$ and $n_90-n_{tr}$ at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm. for PS Run No. 9 at gas pressure of 13.79 MPa.
It can be considered that the gas pressure played a minor role in the measured birefringence distribution of $\Delta n$ and $n_{rr}-n_{\theta\theta}$ since, as discussed in Section 6.4.3, during the filling stage, the birefringence developed in the same manner for the three gas pressures employed because the processing conditions were the same prior to gas penetration. Nevertheless, it can be observed that at 28 cm from the sprue entrance, the simulated birefringence $\Delta n$ showed a shoulder that increase with pressure. This is because high gas pressure leads to fast gas penetration. As a consequence, the shear and normal stresses developed during the gas penetration increased when the pressure increased. This in turn increased the birefringence, as discussed in Section 6.4.3. Nonetheless, it is important to mention that for the GAIM moldings obtained under different gas pressures, the measured birefringence did show a shoulder in the solid region but it was not as well defined as showed in simulations.

6.5.5 The Effect of Injection Speed on Birefringence of PS GAIM Moldings.

Figs. 6-91, 6-92, and 6-93 show the measured and simulated residual birefringence $\Delta n$ and $n_{rr}-n_{\theta\theta}$ for PS Runs No. 10, 11, and 12 at injection speed of 1.27 (0.5), 7.62 (3), and 15.24 (6) cm/s (in/s), respectively, at various distances from the sprue entrance: (a) and (b) in the sprue region at 4 and 6.5 cm, (c) and (d) in the primary gas penetration region of the spiral at 11 and 16 cm; and (e) in the solid. Simulations and measurements showed that the maximum value of the measured birefringence $\Delta n$ at the outer wall increased with the injection speed at all the locations analyzed.
Figure 6-91 Measured and simulated birefringence distribution of $\Delta n$ and $n_{00}-n_{tr}$ at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 34 cm. for PS Run No. 10 at injection speed of 1.27 cm/s.
Figure 6-92 Measured and simulated birefringence distribution of $\Delta n$ and $n_{00} - n_{tr}$ at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 34 cm. for PS Run No. 11 at injection speed of 7.62 cm/s.
Figure 6-93 Measured and simulated birefringence distribution of $\Delta n$ and $n_{rr}-n_{00}$ at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 34 cm. for PS Run No. 12 at injection speed of 15.24 cm/s.
Also, the thickness of the frozen-in birefringence layer decreased when the injection speed increased. For an injection speed of 1.27 cm/s, the measured $\Delta n$ showed a maximum at the outer wall, it increased showing a intermediate maximum and then decreased towards the center showing a plateau near the inner wall. At injection speeds of 7.62 and 15.24 cm/s, the behavior of the birefringence was different. It showed a maximum at the outer wall and decreased steeply toward the center showing a plateau.

Simulations agreed qualitatively with measurements, they showed that the maximum of $\Delta n$ at the outer wall increased when injection speed increased. Also, the birefringence $\Delta n$ diminished with the distance from the sprue entrance showing a maximum value in the sprue region, almost a constant value through the spiral region and the lowest value at the solid region of the spiral. Comparing the birefringence at different injection speeds, it can be observed that, at the lowest injection velocity (1.27 cm/s), the measured $\Delta n$ showed a well defined maximum away from the outer wall. This maximum near the outer wall was formed during the filling stage, as discussed in Section 6.4.4, because of the reduction of the cross-sectional area due to the frozen layer that developed with time. The decrease in the thickness of the frozen-in birefringence when the injection speed increased was because high injection speed led to a low filling time and high shear rate which in turn caused the temperature to increase near the mold wall due to viscous heating. These two effects prevented the melt to solidify during the filling stage leading to a thinner frozen-in layer.

The measured birefringence $n_{rr}-n_{\theta\theta}$ was found to be comparable between the three injection speeds employed. The magnitude of both the measured and simulated flow-induced birefringence $n_{rr}-n_{\theta\theta}$ was significantly lower than the magnitude of the measured
and simulated flow-induced $\Delta n$. Measurements and simulations showed that the thickness of the frozen-in birefringence layer decreased when the injection speed increased. This findings were in agreement with the results showed by Wimberger-Friedl in compact discs of PC [61]. He found that the frozen layer increased by reducing the injection speed and/or the mold temperature.

6.5.6 The Effect of Gas-Delay Time on Birefringence of PS GAIM Moldings.

Figs. 6-94, 6-95, and 6-96 show the measured and simulated residual birefringence $\Delta n$ and $n_{rr} - n_{\theta \theta}$ with respect to the radius for PS Runs No. 13, 14, and 15 at gas-delay times of 0, 3, and 6 s, respectively, at different distances from the sprue entrance: (a) and (b) in the sprue region at 4 and 6.5 cm, (c) and (d) in the primary gas penetration region of the spiral at 11 and 16 cm, and (e) in the solid region. When no gas-delay time was employed to make the samples, the measured birefringence $\Delta n$ showed a maximum near the outer wall, then it decreased towards the inner wall showing a plateau. When gas-delay time was employed, measured $\Delta n$ showed a maximum further away from the outer wall. This maximum of $\Delta n$ was more prominent in the sprue region, as observed in Figs. 6-95a and 6-96a. At gas-delay time of 3 s, the magnitude of the maximum had its highest value in the sprue region. During the primary gas penetration region in the spiral, the magnitude of the maximum was lower and its position was closer to the outer wall. It is important to note that, at certain locations, the maximum of the measured $\Delta n$ showed two peaks (e.g. Fig. 6-96a and b). This was probably caused by a hesitation of the gas during the penetration stage.
Figure 6-94 Measured and simulated birefringence distribution of \( \Delta n \) and \( n_{00}-n_{rr} \) at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm. for PS Run No. 13 at gas-delay time of 0 s.
Figure 6-95 Measured and simulated birefringence distribution of $\Delta n$ and $n_{tr} - n_{00}$ at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 32 cm. for PS Run No. 14 at gas-delay time of 3 s.
Figure 6-96 Measured and simulated birefringence distribution of $\Delta n$ and $n_{00} - n_{\pi\pi}$ at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 32 cm. for PS Run No. 15 at gas-delay time of 6 s.
When the gas-delay time increased, the maximum of the measured $\Delta n$ shifted toward the inner wall of the molding. Simulations showed that this maximum was formed during the gas penetration, as discussed in Section 6.4.5. Simulations also showed that the maximum shifted towards the inner wall when the gas-delay time increased. This is because, the birefringence relaxed rapidly in the core during the delay time. For a specific delay time, as time progressed, the frozen-in layer grew towards the center of the molding creating a zone of low birefringence near the outer wall.

When the gas penetrated, the high viscosity of the polymer in this zone prevented the polymer to flow and the birefringence did not build-up. Therefore, the polymer located in the core, whose temperature was well above $T_g$, flowed during the gas penetration generating shear and normal stresses that build-up the birefringence. When the gas cored-out the polymer, the birefringence relaxed faster near the newly formed inner wall creating the intermediate maximum. The low-birefringence zone increased when the gas-delay time increased. As a consequence, the intermediate maximum shifted towards the center of the molding.

6.5.7 The Effect of Mold Temperature on Birefringence of PS GAIM Moldings.

Figs. 6-97 and 6-98 show the measured and simulated residual birefringence $\Delta n$ and $n_{rr}-n_{\theta\theta}$ for PS Runs No. 16 and 17 at mold temperatures of 30 and 60 °C, respectively, at different distances from the sprue entrance: (a) and (b) in the sprue region at 4 and 6.5 cm, (c) and (d) in the primary gas penetration of the spiral at 11 and 16 cm, and e) in the solid region. The measured birefringence $\Delta n$ and $n_{rr}-n_{\theta\theta}$ for mold temperature of 30 and 60 °C showed a maximum value at the outer wall. Then, both components decreased
Figure 6-97 Measured and simulated birefringence distribution of $\Delta n$ and $n_{tr}-n_{qr}$ at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 32 cm for PS Run No. 16 at mold temperature of 30 ºC.
Figure 6-98 Measured and simulated birefringence distribution of $\Delta n$ and $n_{rr}-n_{00}$ at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm. for PS Run No. 17 at mold temperature of 60 ºC.
towards the inner wall showing a plateau. The magnitude of the maximum $\Delta n$ near the outer wall had a similar magnitude. However, the measured birefringence near the outer wall at the mold temperature of 30 °C showed a thicker frozen-in birefringence layer. This was observed mainly at the transition between the maximum value at the wall and the plateau near the inner wall. The increase of the frozen-in layer thickness corresponded to an increase of the frozen layer developed during the filling stage caused by the lower mold temperature.

The simulated flow-induced birefringence showed a small increase of the maximum of $\Delta n$ at the outer wall. Furthermore, the thickness of the layer where $\Delta n$ is frozen-in increased when the mold temperature decreased. In the solid region, the simulated flow-induced birefringence showed a shoulder that decreased when the mold temperature increased. Furthermore, this shoulder was wider for the mold temperature of 30 °C, due to the faster cooling. The present observations agreed with those made by Isayev and Crouthamel [158] and demonstrated theoretically by Isayev and Hieber [81] that the flow-induced stresses, which are closely related with the flow-induced birefringence, were slightly influenced by an increase in the mold temperature.

6.6 The Effect of Processing Conditions on Birefringence of PC GAIM Moldings

Figs. 6-99, 6-100, and 6-101 show the measured and simulated flow-induced $\Delta n$ and $n_{rr}-n_{\theta\theta}$ for PC Runs No. 1, 2, and 3 at injection speeds of 2.54 (1), 7.62 (3), and 15.24 (6) cm/s (in/s), respectively, at melt temperature of 280 °C at various distances from the sprue entrance: (a) in the sprue region at 4 cm, (b) in the primary gas penetration region of the spiral at 16 cm, and (c) in the solid region. For the three injection speeds, at 4 cm
Figure 6-99 Measured and simulated birefringence distribution of $\Delta n$ and $n_{rr}-n_{00}$ at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 60 cm for PC Run No. 1 at injection speed of 2.54 cm/s and melt temperature of 280 °C.
Figure 6-100 Measured and simulated birefringence distribution of $\Delta n$ and $n_{rr} - n_{00}$ at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 48 cm for PC Run No. 2 at injection speed of 7.62 cm/s and melt temperature of 280 °C.
Figure 6-101 Measured and simulated birefringence distribution of $\Delta n$ and $n_{rr} - n_{\theta\theta}$ at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 48 cm for PC Run No. 3 at injection speed of 15.24 cm/s and melt temperature of 280 °C.

From the sprue entrance, the measured $\Delta n$ showed a positive maximum near the outer wall. Then, it decreased towards the inner wall showing a plateau. Furthermore, at this specific location, the measured $\Delta n$ near the inner wall was significantly higher than the measured $n_{rr} - n_{\theta\theta}$. At the location of 16 cm from the sprue entrance, the magnitude of the measured $\Delta n$ and $n_{rr} - n_{\theta\theta}$ were similar. Then, both birefringence components decreased...
towards the inner wall passing through zero to a negative minimum. After that, the birefringence increased passing once more through zero to a positive maximum near the inner wall. In the solid region, measured $\Delta n$ and $n_{rr}-n_{\theta\theta}$ also showed a positive maximum near the outer wall, they decreased passing through zero to a negative minimum. Then $\Delta n$ and $n_{rr}-n_{\theta\theta}$ increase passing through zero once more to an extensive positive region in the core. It is important to note that the position at which the birefringence changed from positive to negative, shifted towards the outer wall when the injection speed increased. This was because the thickness of frozen-in layer decreased with injection speed.

The simulated flow-induced birefringence near the outer wall, increased when the injection speed increased. Furthermore, the thickness of the simulated frozen-in birefringence decreased when the injection speed increased, as discussed in Section 6.4.4.

Figs. 6-102, 6-103, and 6-104 show the measured and simulated residual birefringence $\Delta n$ and $n_{rr}-n_{\theta\theta}$ for PC Runs No. 4, 5, and 6 at injection speeds of 2.54 (1), 7.62 (3), and 15.24 (6) cm/s (in/s), respectively, at melt temperature of 300 °C at various distances from the sprue entrance: (a) in the sprue region at 4 cm, (b) in the primary gas penetration region of the spiral at 16 cm, and (c) in the solid region. At the location of 4 cm, the measured birefringence near the outer wall decreased when the injection speed increased. This is because the layer of the frozen-in birefringence became thinner when the injection speed increased and the birefringence further away from this layer relaxed. Therefore, the value of $\Delta n$ measured away from the outer wall decreased. The birefringence close to the outer wall was not possible to measure. For the location of 16 cm, the position where the measured birefringence changed from positive to negative
shifted to the outer wall. Simulated flow-induced birefringence, $\Delta n$ and $n_{rr} - n_{\theta\theta}$, increased with the injection speed.

![Graph a) Measured $\Delta n$ and $n_{rr} - n_{\theta\theta}$](image_a)

![Graph b) Measured $\Delta n$ and $n_{rr} - n_{\theta\theta}$](image_b)

![Graph c) Measured $\Delta n$ and $n_{rr} - n_{\theta\theta}$](image_c)

Figure 6-102 Measured and simulated birefringence distribution of $\Delta n$ and $n_{rr} - n_{\theta\theta}$ at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 60 cm for PC Run No. 4 at injection speed of 2.54 cm/s and melt temperature of 300 ºC.
Figure 6-103 Measured and simulated birefringence distribution of $\Delta n$ and $n_{rr}-n_{00}$ at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 60 cm for PC Run No. 5 at injection speed of 7.62 cm/s and melt temperature of 300 ºC.
Figure 6-104 Measured and simulated birefringence distribution of $\Delta n$ and $n_{rr} - n_{00}$ at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 60 cm for PC Run No. 6 at injection speed of 15.24 cm/s and melt temperature of 300 ºC.

Figs. 6-105, 6-106, and 6-107 show the measured and simulated birefringence $\Delta n$ and $n_{rr} - n_{00}$ for PC Runs No. 7, 8, and 9 at injection speeds of 2.54 (1), 7.62 (3), and 15.24 (6) cm/s (in/s), respectively, at melt temperature of 320 ºC at various distances from the sprue entrance: (a) in the sprue region at 4 cm, (b) in the primary gas penetration region of the spiral at 16 cm, and (c) in the solid region. In general, simulations and experiments
showed that the birefringence near the outer wall decreased when the temperature increased. It is important to note that at temperature of 320 ºC, the negative minimum of the birefringence at 16 cm from the sprue entrance decreased with respect to that observed at low melt temperature.

Figure 6-105 Measured and simulated birefringence distribution of $\Delta n$ and $n_{rr}-n_{\theta\theta}$ at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 60 cm for PC Run No. 7 at injection speed of 2.54 cm/s and melt temperature of 320 ºC.
Figure 6-106 Measured and simulated birefringence distribution of $\Delta n$ and $n_{rr}-n_{00}$ at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 60 cm for PC Run No. 8 at injection speed of 7.62 cm/s and melt temperature of 320 °C.
It is important to note that, for a specific injection speed, the simulated birefringence decreased when the melt temperature increased. This is because, as discussed in Section 6.4.1, the viscosity and the relaxation time decreased when the temperature increased, which leads to a lower birefringence.
The maximum value of birefringence near the outer wall decreased when the injection speed increased. This is because the frozen layer became thinner and the location where the birefringence was measured corresponded to a location where the birefringence could relax due to the high temperature, as explained in Section 6.4.4. It is important to note that the measured birefringence \( n_{rr} - n_{\theta\theta} \) near the inner wall was higher than the measured birefringence \( \Delta n \). This effect was observed in the free quenching experiments to be discussed in Chapter VII.

6.7 Effect of Processing Conditions on Average Birefringence of PS GAIM Moldings

The following sections present the effect of processing conditions on the measured and simulated average birefringence \( \langle n_{zz} - n_{\theta\theta} \rangle \). Measurements and simulations of \( \langle n_{zz} - n_{\theta\theta} \rangle \) were carried out in the spiral moldings at various distances from the sprue entrance.

6.7.1 The Effect of Melt Temperature on Average Birefringence of PS GAIM Moldings.

Fig. 6-108 shows the measured and simulated average birefringence \( \langle n_{zz} - n_{\theta\theta} \rangle \) for Runs No. 1, 2, and 3 at melt temperatures of 180, 200, and 230 °C, while the rest of the processing variables were held constant. At the three melt temperatures, the measured birefringence \( \langle n_{zz} - n_{\theta\theta} \rangle \) decreases along the sprue length and along the primary and secondary gas penetration regions of the spiral. It showed a short plateau in the primary gas penetration region of the spiral and it remained almost constant in the solid region. Clearly, the overall magnitude of the average birefringence \( \langle n_{zz} - n_{\theta\theta} \rangle \) decreased along the whole length of the molding when the melt temperature increased. This behavior was
caused by a decrease in the relaxation time when the melt temperature increased. Additionally, for melt temperatures of 200 and 230 °C, the measured average birefringence exhibited a minimum between the plateaus of the primary gas penetration and the solid regions of the spiral. This minimum can be attributed both the proximity of the solid region where high temperature could have led to a relaxation of stresses and birefringence in this region. It was also possible that the slow progress of the gas front could have caused biaxial stretching leading to a different molecular orientation at the inner wall. Nevertheless, a detailed study of this region’s birefringence must be carried out in order to elucidate this effect.

Figure 6-108 Measured and simulated average birefringence $<n_{zz} - n_{θθ}>$ with respect to the distance from the sprue entrance for PS Runs No. 1, 2, and 3 carried out at different melt temperatures.

Simulations showed qualitatively the effect of melt temperature on the average birefringence $<n_{zz} - n_{θθ}>$. The simulated average birefringence showed that $<n_{zz} - n_{θθ}>$ decreased along the sprue, showed a plateau along the primary gas penetration region of
the spiral and decreased to almost a constant value in the solid region. Furthermore, the overall magnitude of the simulated $<n_{zz} - n_{\theta\theta}>$ decreased along the spiral when the melt temperature increased. However, the simulations carried out at melt temperatures of 180 and 200 °C showed a higher magnitude of $<n_{zz} - n_{\theta\theta}>$ than the corresponding measured one. However, the simulation carried out at 230 °C shows a lower magnitude of $<n_{zz} - n_{\theta\theta}>$ with respect to the measured one in the primary gas penetration of the spiral. The deviation between the measurements and simulations of $<n_{zz} - n_{\theta\theta}>$ can be attributed to over-prediction of the flow-induced birefringence as discussed in Section 6.5.2.

6.7.2 The Effect of Shot Size on the Average Birefringence of PS GAIM Moldings

Fig. 6-109 shows the measured and simulated average birefringence $<n_{zz} - n_{\theta\theta}>$ with respect to the distance from the sprue entrance for PS Runs No. 4, 5, and 6 at different shot sizes of 75, 85, and 90%, while the rest of the processing variables were held constant. At shot sizes of 75 and 85%, the measured average birefringence $<n_{zz} - n_{\theta\theta}>$ decreased along the sprue and showed a plateau in the primary gas penetration region of the spiral. After that, it decreased and remained almost constant in the solid region leading to the second plateau region. At shot sizes of 75 and 85%, the measured average birefringence showed practically the same magnitude in the primary gas penetration region of the spiral, even though the length of the primary gas penetrations was substantially longer at shot size of 75%. Also, at both shot sizes, 75 and 85%, a minimum between the two plateaus was observed. At the shot size of 90% the gas penetrated the length of the sprue but barely penetrated the spiral. For this reason, the birefringence throughout the length of the spiral behaved like that observed in the solid region. One can
see that the shot size has a significant influence on the birefringence distribution in the length direction.

Figure 6-109 Measured and simulated average birefringence $<n_{z} - n_{θθ}>$ with respect to the distance from the sprue entrance for PS Runs No. 4, 5, and 6 carried out at different shot sizes.

Simulations showed that the average birefringence plateau in the primary gas penetration region enlarged when the shot size decreased. However, the simulated average birefringence at shot size of 75% showed a lower magnitude of the birefringence plateau in the primary gas penetration than that at the shot sizes of 85 and 90%. The reason for the decrease was that the predicted RWT at the shot size of 75% was slightly thicker than the simulated RWT at shot sizes of 85 and 90%.

6.7.3 The Effect of Gas Pressure on Average Birefringence of PS GAIM Moldings

Fig. 6-110 shows the measured and simulated average birefringence, $<n_{z} - n_{θθ}>$, with respect to the distance from the sprue entrance for PS Runs No. 7, 8, and 9 at gas
injection pressures of 6.89 (1000), 10.34 (1500), and 13.79 MPa (2000 psi), while the rest of the processing variables were held constant. The measured average birefringence at the gas pressure of 6.89 MPa was lower all along of the molding than the measured average birefringence at the gas pressure of 10.34 MPa. The average birefringence in the primary gas penetration region of the spiral at the gas pressure of 13.79 MPa could not be measured due to the presence of microbubbles at the polymer/gas interface. These microbubbles impeded passage of light through the diameter of the sample. The formation of the microbubbles was apparently caused by the high gas pressure. Nevertheless, the measured birefringence in the sprue region at the gas pressure of 13.79 MPa shows a similar value as that at gas pressure of 10.34 MPa, while the birefringence in the solid region, exhibited an intermediate value between the average birefringence at gas pressures of 6.89 and 10.34 MPa.

![Diagram](image_url)

**Figure 6-110** Measured and simulated average birefringence $<n_{zz}>-n_{θθ}$ with respect to the distance from the sprue entrance for PS Runs No. 7, 8, and 9 carried out at different gas pressures.
Simulations showed that the overall magnitude of the simulated average birefringence increased with the gas pressure. This is because of the increase of shear and normal stresses generated during the gas penetration stage. The increase of the simulated $<n_{zz}-n_{θθ}>$ with an increase of the gas pressure was more noticeable in the primary gas penetration of the sprue and spiral regions than that in the solid region. This was because the RWT decreased when the gas pressure increased in regions where the gas cored out the polymer. Thus, the average birefringence was influenced by the RWT. In the solid region, the increment of the simulated $<n_{zz}-n_{θθ}>$ was due solely to the increase of shear and normal stresses when the gas pressure increased.

6.7.4 The Effect of Injection Speed on Average Birefringence of PS GAIM Moldings

Fig. 6-111 shows the measured and simulated average birefringence, $<n_{zz}-n_{θθ}>$, with respect to the distance from the sprue entrance for PS Runs No. 10, 11, and 12, at injection speed of 1.27 (0.5), 7.62 (3), and 15.24 cm/s (6 in/s) while the rest of the processing variables were held constant. The measured average birefringence at injection speeds of 1.27 and 7.62 cm/s in the primary gas penetration region had practically the same magnitude. For the injection speed of 15.24 cm/s, the average birefringence was higher than that for injection speeds of 1.27 and 7.62 cm/s. In the solid region, the measured $<n_{zz}-n_{θθ}>$ for injection speed of 1.27 cm/s was higher than that for 7.62 and 15.24 cm/s. The latter two speeds showed similar values of birefringence. The measured average birefringence for injection speed of 1.27 cm/s showed a longer plateau in the primary gas penetration region because of the increase of the gas penetration length when the injection speed decreased.
Simulations showed that along the sprue the birefringence $<n_{zz} - n_{θθ}>$ increased when the injection speed decreased. However, the birefringence in the primary gas penetration region of the spiral showed almost a constant plateau at the three injection speeds. In the solid region, the simulated average birefringence increased when the injection speed decreased. Also, it can be observed that the simulated average birefringence, at low injection speed, showed a longer plateau in the gas penetration region of the spiral than the other two velocities, due to the increase in the gas penetration.

It is important to observe that the average birefringence in the sprue, was the highest for the injection speed of 1.27 cm/s (Run No. 10). This is because, at low injection speed, the birefringence developed near the wall gets frozen-in by the temperature drop near the mold wall. Low injection speed created a thick frozen-in...
birefringence layer, as observed in Fig. 6-91. This effect was more evident in the sprue region (Fig. 6-91a) where the flow-induced birefringence was higher since the diameter of the sprue is considerably lower than that of the spiral region.

6.7.5 The Effect of Gas-Injection-Delay Time on the Average Birefringence of PS GAIM Moldings

Fig. 6-112 shows the measured and simulated average birefringence \(<n_{zz}-n_{\theta\theta}\rangle\) distribution along the flow direction for PS Runs No. 13, 14, and 15, at gas-injection-delay time of 0, 3, and 6 s while the rest of the processing variables were held constant. The measured average birefringence along the sprue and in the primary gas penetration region of the spiral decreased when the gas-delay time increased. Furthermore, at gas delay-time of 6 s the length of the plateau of the measured average birefringence in the primary gas penetration region of the spiral was shorter than that at gas-delay time of 3 s, since at gas-delay time of 6 s the mold was not completely filled and the gas penetration length was shorter than that of gas-delay time of 3 s, as explained in Section 6.2.5. In the solid region of the spiral, the magnitude of the measured average birefringence was similar at the three gas-delay times. The decrease of the average birefringence when the gas-delay time increased was attributed to the increase of the RWT with gas-delay time. This is because when the retardation of the polarized light was averaged along the wall thickness the magnitude of the average birefringence was lower. Simulations qualitatively described the effect of the gas-delay time on the average birefringence \(<n_{zz}-n_{\theta\theta}\rangle\). The overall magnitude of \(<n_{zz}-n_{\theta\theta}\rangle\) decreased along the length of the molding when the gas-delay time increased.
Figure 6-112 Measured and simulated average birefringence \(<n_{zz} - n_{\theta \theta}>\) with respect to the distance from the sprue entrance for PS Runs No. 13, 14, and 15 carried out at different delay times.

This was attributed to both the birefringence relaxation in the core region during the delay time and the increase of the wall thickness with gas-delay time. Thicker wall thickness renders a lower averaged value of birefringence.

6.7.6 The Effect of Mold Temperature on the Average Birefringence of PS GAIM Moldings

Fig. 6-113 shows the measured and simulated average birefringence \(<n_{zz} - n_{\theta \theta}>\) distribution along the flow direction for PS Runs No. 16 and 17, at mold temperature of 30 and 60 °C, while the rest of the processing variables were held constant. It was observed that the overall magnitude of the measured average birefringence increased when the mold temperature decreased. This is because lower mold temperatures led to a thicker frozen-in layer of the flow-induced birefringence. This led to a higher magnitude
of the retardation, and as a consequence the average birefringence increased. Simulations also showed that the average birefringence increased when mold temperature decreased. This is because the birefringence $n_{zz} - n_{θθ}$ increased along the radius.

![Graph showing the relationship between mold temperature and average birefringence](image)

Figure 6-113 Measured and simulated average birefringence $<n_{zz} - n_{θθ}>$ with respect to the distance from the sprue entrance for PS Runs No. 16 and 17 carried out at different mold temperatures.

6.8 The Effect of the Injection Speed on Average Birefringence of PC GAIM Moldings

Fig. 6-114 shows the measured and simulated average birefringence, $<n_{zz} - n_{θθ}>$, distribution along the flow direction for PC Runs No. 1, 2, and 3 at injection speeds of 2.54, 7.62, and 15.24 cm/s. The measured birefringence decreased with respect to the distance from the sprue entrance. Then, it showed a plateau in the primary gas penetration region of the spiral. In the solid region, the measured average birefringence showed a higher value than that of the primary gas penetration of the spiral.
The simulated flow-induced average birefringence decreased with the distance from the sprue entrance. It remained almost constant in the primary gas penetration of the spiral, and decreased significantly in the solid region. The simulated average birefringence in the spiral increased with the injection speed. It is important to note that the measured average birefringence was higher than the simulated flow-induced average birefringence. It is important to mention that the contribution of the simulated thermally-induced birefringence was not included in Fig. 6-114. It will be discussed in Chapter VIII. Furthermore, the average birefringence for PC Runs No. 4 to 9 could not be measured, due to microbubbles on the polymer/gas interface that impeded the passage of light through the diameter of the moldings.
6.10 Birefringence in Annealed Sample of PS

It was believed that the birefringence away from the outer wall was mainly due to cooling effect. In order to verify this hypothesis, a sample of 4 cm long from a GAIM spiral of Run No. 18 was annealed at 88 °C in an oven for 1 hour. The annealing temperature and time were selected based on experiments carried out at several temperatures. At higher temperature the birefringence near the wall decreased and the dimensions of the sample changed considerably. However, after annealing the sample at 88 °C, no appreciable changes in its dimensions were observed. The sample was sliced and the birefringence measured according to the procedure described in Section 5.3. Fig. 6-115 shows the radial distribution of birefringence (a) $\Delta n$ and (b) $n_{rr} - n_{\theta\theta}$ along the wall thickness before and after annealing at distances of 35 and 37 cm from sprue entrance, respectively. One can compare the birefringence distributions at these two locations in proximity of each other, since $\Delta n$ and $n_{rr} - n_{\theta\theta}$ behave similarly in the primary gas penetration region of the spiral. After annealing, $\Delta n$ did not relax at the outer wall, while at the inner wall, it relaxed significantly. Also, although the maximum located further away from the wall reduced in its value, it did not disappear. Similar to $\Delta n$, $n_{rr} - n_{\theta\theta}$ component showed almost no relaxation at the outer wall, but at its minimum at $r/R = 0.82$ increased. Also, this component showed a plateau towards the inner wall. This behavior could indicate that the birefringence near the outer wall was caused by the shear and normal stresses during cavity filling and gas penetration, while the birefringence near the inner wall is caused by thermal stresses during solidification which can relax at temperatures near the glass transition temperature. It is important to note that the birefringence $n_{rr} - n_{\theta\theta}$ (Fig. 6-115b) (about $r/R=0.8$) increased after the sample was
annealed. This could have been caused by a redistribution of stresses when the slice used to measure the birefringence was removed from the annealed sample.

Figure 6-115 Measured radial distribution of birefringence $\Delta n$ (a) and $n_{rr}-n_{00}$ (b) in primary gas penetration region of the spiral at 35 cm from the sprue entrance before annealing ($\circ$) and at 37 cm after annealing at 88 ºC for 1 hour ($\times$).

6.10 Birefringence in Annealed Sample of PC

In order to verify the hypothesis made in the preceding section for the birefringence of PC GAIM moldings, a section of 4 cm of a PC GAIM molding of Run No. 1 was immersed in silicon oil and annealed at 140 ºC for 12 hours. The temperature and time were selected based on preliminary experiments. Higher annealing temperature caused the birefringence to relax almost completely and there were detectable differences in the sample’s dimensions. However, after annealing the section of PC at 140 ºC, no changes in the sample’s dimensions were detected. Then, the annealed sample was sliced and the birefringence was measured according to the procedure described in Section 5.3. Fig. 6-116 shows the radial distribution of birefringence (a) $\Delta n$ and (b) $n_{rr}-n_{00}$ along the
wall thickness before and after annealing at distances of 35 and 37 cm from sprue entrance, respectively. For the annealed samples of PC, it was found that the birefringence components $\Delta n$ and $n_{rr}-n_{\theta\theta}$ relaxed significantly near both the outer and inner walls.

This could be an indication that, for the case of PC GAIM moldings, the birefringence near the outer wall was also introduced by thermal stresses during cooling. Similar to the PS GAIM moldings, it was observed that the birefringence $n_{rr}-n_{\theta\theta}$ at the location of $r/R=0.8$ increased after annealing the sample. This could have been caused by a redistribution of stresses upon relieving the thermally-induced stresses. The effect of thermally-induced birefringence will be discussed in Chapters VII and VIII.
6.11 Conclusions

The effect of the processing conditions on the polymer/gas interface distribution were measured and simulated for PS and PC GAIM tubular moldings. In general, the most important processing parameters that strongly influence the gas penetration length and the RWT in PS GAIM moldings were the injection speed and the gas-delay time. The shot size exerted a definite influence on the gas penetration length, however, the RWT only increased when the shot size was large (i.e. 90%). The processing parameters that exerted less influence on gas penetration length and the RWT, were the gas pressure, the melt and mold temperature. Simulations qualitatively described the effect of the processing conditions on the gas penetration length and RWT.

Furthermore, the radial distribution of birefringence $\Delta n$ and $n_{rr} - n_{\theta\theta}$ and the average birefringence $<n_{zz} - n_{\theta\theta}>$ were measured and the corresponding flow-induced birefringence simulated for PS and PC GAIM moldings. It was found that the measured birefringence components $\Delta n$ and $n_{rr} - n_{\theta\theta}$ showed a maximum near the outer wall of the molding. This maximum decreased along the sprue, remained almost constant in the primary gas penetration of the spiral, and decreased in the solid region. Simulations qualitatively described the measurements. However, it was found that for the case of PS, the simulated $\Delta n$ was higher than the measured $\Delta n$. This effect was attributed to the over-prediction of cooling, due to the assumption made about the constant mold temperature.

The influence of the processing variables on the simulated transient flow-induced birefringence $\Delta n$ was presented. Simulations showed that the maximum of $\Delta n$ near the outer wall was caused by shear and normal stressed generated during the filling stage. The birefringence near the inner wall and in the core region (for the solid section),
partially relaxed during the gas penetration stage. However, the displacement of the polymer at the core prevented the birefringence to relax completely. When the gas cored out the polymer, the birefringence near newly formed inner wall relaxed due to the elevated melt temperature in this region.

The influence of the processing variables on the average birefringence $<n_{zz}-n_{θθ}>$ along the molding length was elucidated. Measurements and simulations showed that, for PS GAIM moldings, the average birefringence decreased along the sprue, it showed a plateau in the primary gas penetration region of the spiral, and decreased in the solid region of the spiral. Conversely, for PC GAIM moldings, it was found that the measured average birefringence decreased along the sprue, remained almost constant along the primary gas penetration, and increased in the solid region. The simulated average birefringence did not describe completely the measured average birefringence in PC GAIM moldings because the contribution of the thermally-induced average birefringence was not taken into account in this section. The contribution of the thermally-induced average birefringence in GAIM moldings will be added to the average birefringence induced by flow to obtain the total average birefringence. This will be discussed in Chapter VIII.

The most important parameters that strongly influenced the average birefringence in PS GAIM moldings was the melt temperature, followed by the gas-delay time and injection speed. The shot size and the gas pressure were the processing variables that exerted less influence on the average birefringence.

When a section of a PS GAIM molding was annealed at 88 ºC for 1 hour, the measured birefringence $Δn$ and $n_{rr}-n_{θθ}$ near the outer wall did not relax while the
birefringence near the inner wall relaxed. However, when a section of a PC GAIM molding was annealed at 140 °C for 12 hours. The measured birefringence $\Delta n$ and $n_{rr} - n_{\theta\theta}$ relaxed significantly at both the inner and outer walls. This was an indication that, for PC GAIM moldings the thermally-induced birefringence exerted a strong influence throughout the RWT.

It was found that for the PS GAIM moldings, the thickness of the slices cut from the GAIM moldings to measure the birefringence did not altered significantly the birefringence distribution. However, for PC GAIM moldings, the thickness of the slices was critical. It was found that thin slices altered significantly both $\Delta n$ and $n_{rr} - n_{\theta\theta}$ distribution.
CHAPTER VII
THERMALLY-INDUCED RESIDUAL STRESSES AND BIREFRINGENCE:
SIMULATION AND EXPERIMENT

This chapter presents measurements and simulations of the radial distribution of thermally-induced residual birefringence, $\Delta n$ and $n_{rr}-n_{\theta \theta}$, and the average birefringence, $\langle n_{zz}-n_{\theta \theta} \rangle$, in free quenched tubes and rods of PS and PC. Furthermore, the simulated distribution of transient and residual thermally-induced stress components in radial, circumferential, and axial directions of free quenched tubes and rods are analyzed. The objective of the experiments and simulations was to elucidate the contribution of thermal stresses on the residual birefringence in gas-assisted injection moldings. Simulations of stresses and birefringence components were based, respectively, on linear viscoelastic and photoviscoelastic theories according to the derivation presented in Chapter IV.

7.1 Experimental Procedure for Free Quenching of Tubes and Rods

Free quenching experiments were carried out on tubes and rods of PS and PC at different initial temperatures. The samples of PS were quenched from 105, 120, and 135 °C in water at 25 °C. The samples of PC were quenched from 170 and 180 °C in water at 25 °C. To obtain the samples, rods having a length of 60 mm and a diameter of 10 mm were fabricated by melting separately PS and PC pellets into a cylindrical mold heated in a vacuum oven at 200 °C and 250 °C for two hours, respectively. To obtain the tubular
samples, the rods were axially drilled to a diameter of 5 mm. In order to eliminate the residual birefringence introduced during the fabrication and/or drilling processes, the samples of PS and PC were immersed in silicon oil and annealed, respectively, at 105 °C and at 155 °C for 10 hours. Subsequently, the samples were cooled slowly. After the annealing, the samples’ average residual birefringence, \(<n_{zz}-n_{θθ}>\), was negligible (of the order of 10^{-7}).

Prior to the quenching experiments, both ends of the tubes were sealed in order to avoid ingress of water to its interior. The purpose of this was to remove the heat through the outer wall of the sample in order to mimic the GAIM process, where the sample’s heat was removed through the surface that was in contact to the mold wall. To perform the quenching, the samples were placed vertically in an oven at the specified initial temperature for 15 minutes. Afterward, the samples were submerged vertically into water at 25±1 °C. The cylindrical coordinate system (z, r, θ) was used to identify the sample’s axial, radial, and circumferential directions, respectively. The distribution of the birefringence components, \(Δn\) and \(n_{rr}-n_{θθ}\), and the average birefringence, \(<n_{zz}-n_{θθ}>\), were measured two days after the quenching experiments according to the procedure described in the Section 5.3. The thickness of the slices was 1 mm in the plane z-r and 2 mm in the plane r-θ, unless otherwise specified.

7.2 Transient Thermal Stresses for an Ideal Elastic Tube

This section discusses the analytical and numerical solutions of thermal stresses induced by a temperature gradient on elastic tube whose material properties are independent of temperature and time. The results presented here are useful to explain the
evolution of thermal stresses in viscoelastic materials whose properties depend on time and temperature. Thermal stresses are induced by inhomogeneous contraction due to a temperature gradient. Fig. 7-1 shows both the analytical (a) (Eqs. 7-1, 7-2, and 7-3) [123] and the numerical solutions (a) (Eqs. 4-31, 4-32, and 4-33) of thermal stress components in radial (σ_{rr}), tangential (σ_{θθ}), and axial (σ_{zz}), directions for an elastic tube quenched from 120 °C to 25 °C at 22 s after the beginning of quenching. The analytical solution of thermal stresses in a tube with an arbitrary temperature (T) along the radius (r) is given by [123]:

\[
\sigma_{rr} = \frac{\alpha E}{1 - \nu} \frac{1}{r^2} \left( \frac{r^2 - a^2}{b^2 - a^2} \int_a^b T r dr - \int_a^b T r dr \right)
\]

(7-1)

\[
\sigma_{θθ} = \frac{\alpha E}{1 - \nu} \frac{1}{r^2} \left( \frac{r^2 + a^2}{b^2 - a^2} \int_a^b T r dr - \int_a^b T r dr - T r^2 \right)
\]

(7-2)

\[
\sigma_{zz} = \frac{\alpha E}{1 - \nu} \left( \frac{2}{b^2 - a^2} \int_a^b T r dr - T \right)
\]

(7-3)

where \(a\) and \(b\) represent the inner and outer radii of the tube, \(E\) is the Young’s modulus and \(\nu\) is the Poisson ratio.

For this specific example, the shear modulus was considered constant and equal to the shear modulus of the PS at 25 °C (2.3 GPa). The dimensions of the elastic tube were identical to those of the actual tubular samples used for quenching experiments. The numerical simulations were performed using 40 nodes along the radius and a constant time step of 0.1 s. The heat transfer coefficient employed in for this example was \(h=490\) J/s m\(^2\) K.

The values of stresses obtained from analytical and numerical calculations for an elastic tube were the same. The radial stresses, \(σ_{rr}\), were compressive throughout the
radius and zero at the inner and outer surfaces of the tube, as required by the traction free boundary condition. The axial, \(\sigma_{zz}\), and circumferential, \(\sigma_{\theta\theta}\), stresses were tensile near the outer wall, and they decrease passing through zero to a negative region near the inner wall.

**Figure 7-1** Analytical (a) and numerical (b) solutions of transient thermal stresses for an elastic cylinder at 22 s after the beginning of quenching.

Fig. 7-2 shows the numerical simulation of transient thermal stresses for the elastic tube. At the beginning of cooling, the external layers of the cylinder contracted and compressed the inner layers of the cylinder. Since the Young’s modulus throughout the radius was constant, there was no stress relaxation and the stress equilibrium was balanced throughout the wall thickness. During the cooling, the radial stresses were compressive throughout the wall and zero at the inner and outer wall surfaces, as required by the traction-free boundary condition. The circumferential and axial stresses were always in tension near the outer wall, where they showed their highest value. Then, they
decrease passing through zero to a negative value (compression), showing a highest value at the inner wall.

Figure 7-2 Simulated transient thermal stresses in an elastic tube quenched from 120 to 25 ºC.

As the cooling progressed, the circumferential and axial stresses at the inner and outer walls reached a maximum in time and decreased as the temperature gradient reduced. When the tube’s temperature was uniform, the stresses vanished, as observed in Fig. 7-2 at 400 s.
7.3 Instability of the Code

It was found that the quasi-static approximation presented in Chapter IV to calculate the stresses and residual birefringence was unstable. This is because the modulus of the polymer increases by a factor of 1000 in a 20 to 30 °C range when the polymer cools down from above to below $T_g$ [159]. During the quenching process, the fast temperature drop near the outer wall creates a large temperature gradient. When the mesh was coarse, the temperature difference between two adjacent nodes near the outer wall was large. This caused a large difference in the shear modulus since in two consecutive nodes, the temperature of one of them was higher than $T_g$ while in the adjacent node, the temperature could have been below $T_g$. Therefore, the terms that involve derivatives of the modulus became large leading to instabilities. Therefore, it was imperative to refine the mesh in the radial direction. Fig. 7-3 shows the stress calculation for 150, 250, and 500 meshes along the radial direction. It is important to point out that the mesh refinement, in this case, affects the global stability of the code, according to the stability conditions of the space and time derivatives.

It was observed that the stress calculated with 150 meshes showed a large deviation from the parabolic distribution, especially near the outer wall of the cylinder. Also, the birefringence showed a sharp transition from positive to negative and a large negative value near the outer wall. When the number of meshes was increased to 250, the stresses showed a parabolic distribution. The birefringence showed a gradual transition between the positive and negative values and a lower magnitude at the outer wall than that calculated with 150 meshes. When the number of meshes was increased to 500, the stresses and birefringence were closer to the results obtained with 250 meshes.
Figure 7-3 Axial stresses (a) and birefringence $\Delta n$ (b) calculated with various number of meshes along the radius.

Therefore the calculations were performed using 500 meshes with a variable time step listed in Appendix B. The material constants employed in the simulations are reported in Table 7-1.

Table 7-1 Material Constant of PS and PC Used in Simulations

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$\beta_l$</td>
<td>0.00021</td>
<td>0.0002</td>
</tr>
<tr>
<td>$\beta_g$</td>
<td>0.000066</td>
<td>0.00067</td>
</tr>
<tr>
<td>$\alpha$ (m$^2$/s)</td>
<td>6.13x10$^{-8}$</td>
<td>7.31x10$^{-8}$</td>
</tr>
<tr>
<td>Poison ratio</td>
<td>0.33</td>
<td>0.41</td>
</tr>
<tr>
<td>WLF equation:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$C_1$</td>
<td>10.6</td>
<td>8.82</td>
</tr>
<tr>
<td>$C_2$ (K)</td>
<td>57.0</td>
<td>40.2</td>
</tr>
<tr>
<td>$T_1$ (K)</td>
<td>370.0</td>
<td>420.5</td>
</tr>
<tr>
<td>$T_2$ (K)</td>
<td>313.0</td>
<td>380.0</td>
</tr>
<tr>
<td>$\tau_r$</td>
<td>0.04 s at 97 °C</td>
<td>0.3 s at 147 °C</td>
</tr>
<tr>
<td>Thermal properties</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$h$ (J/s m$^2$ K)</td>
<td>490</td>
<td>490</td>
</tr>
</tbody>
</table>

Simulations of free quenching were carried out considering the volume relaxation approach [133]. As a first approximation, a single relaxation time, $\tau_r$, of 0.04 s at a
The reference temperature of 97 °C was employed for PS and a single relaxation time of 0.3 s at a reference temperature of 147 °C for PC. These relaxation times were selected based on free quenching experiments carried out on plates [11].

The relaxation modulus and the strain optical coefficient were measured previously by Shyu [11,102]. The master curves of relaxation modulus, the strain optical coefficient and the reduced time for PS and PC are shown in Figs. 7-4 and 7-5, respectively.

![Figure 7-4 Master curve of Young’s modulus, \( E \), (a), master curve of the strain-optical coefficient, \( C_\varepsilon \), (b), and temperature dependence of the shift factor, \( a_T \), of \( E \) and \( C_\varepsilon \) (c) for PS at a reference temperature of 97 °C [102].](image-url)

Figure 7-4 Master curve of Young’s modulus, \( E \), (a), master curve of the strain-optical coefficient, \( C_\varepsilon \), (b), and temperature dependence of the shift factor, \( a_T \), of \( E \) and \( C_\varepsilon \) (c) for PS at a reference temperature of 97 °C [102].
7.4 Transient Residual Stresses in Viscoelastic Tubes

This section presents the simulated transient thermally-induced stresses and birefringence in PS and PC tubes. Fig. 7-6 shows the simulated transient thermal stresses for a PS tube quenched in water from 120 to 25 °C. These calculations were performed considering the viscoelastic material properties reported in Table 7-1 and the data from
the master curves shown in Figs. 7-4 and 7-5. At the beginning of the quenching, $t=0.35\text{s}$, the polymeric layers near the tube surface shrunk. The contraction of these layers compressed the polymer located toward the inner wall. Due to the force balance along the radius, the outer layers were in tension (Fig. 7-6b and 7-6c at 0.35 s) while the inner layers were in compression. When the temperature of the polymer near the surface dropped below $T_g$, it solidified and its contraction rate decreased. At the early stages of quenching, the high temperature near the inner wall allowed the stresses to relax. As cooling progressed, each layer, as it cooled and contracted, compressed the layers located near the outer wall already solidified. To satisfy the force balance, tensile stresses in the radial direction and compressive axial and circumferential stresses at the surface were created. Along the radius, the axial stresses, $\sigma_{zz}$, were compressive (negative) near the outer wall and tensile in the inner layers. The axial stresses were balanced such that the negative and positive portions were equal, i. e. $\int_0^\rho 2\pi \sigma_{zz} \, dr = 0$.

During the solidification of the inner region of the tube, the stresses build-up maintaining the equilibrium throughout the tube wall. The thermal contraction of the outer layers creates tensile stresses at the surface and compression at the inner layers. This process continued until the temperature through wall thickness became homogeneous rendering the residual stress distribution. After the polymer reached the final equilibrium temperature, the volume relaxation allowed the stresses to relax, as observed in Fig. 7-6 at the time of $2 \times 10^5 \text{s}$.
Figure 7-6 Simulated transient thermal stresses for a PS tube quenched in water from 120 to 25 ºC: a) radial, $\sigma_{rr}$, b) circumferential, $\sigma_{\theta\theta}$, and c) axial, $\sigma_{zz}$.

Fig. 7-7 shows the simulated transient birefringence (a) $\Delta n$ and (b) $n_{rr}-n_{\theta\theta}$ for a PS tube, quenched from 120 to 25 ºC. At the beginning of the quenching (0.35 s), $\Delta n$ and $n_{rr}-n_{\theta\theta}$ showed a negative value near the outer wall, then it decreased passing through zero to a positive value near the inner wall. At high temperature, the strain-optical coefficient of PS is negative [11]. Therefore, at the beginning of the quenching process, the birefringence induced at the surface was negative, since the stresses in this region were
tensile. This caused the birefringence to be negative for PS while the region near the inner wall the stresses were compressive and the birefringence was positive.

![Graph showing simulated transient birefringence](image)

**Figure 7-7** Simulated transient birefringence (a) $\Delta n$ and (b) $n_{rr}-n_{\theta\theta}$ for a polystyrene tube quenched in water from 120 to 25 °C.

Fig. 7-8 shows the simulated transient stress differences, $\sigma_{zz}-\sigma_{rr}$ (a) and $\sigma_{rr}-\sigma_{\theta\theta}$ (b), for a PS tube quenched from an initial temperature of 120 °C to 25 °C. At the early stages of the quenching process (0.35 s), $\sigma_{zz}-\sigma_{rr}$ was positive at the outer wall and negative towards the center. As the cooling progresses, $\sigma_{zz}-\sigma_{rr}$ changed from positive to negative at the surface. Conversely, at the early stages of the quenching process (0.35 s), the stress difference, $\sigma_{rr}-\sigma_{\theta\theta}$, was negative and then changed to a positive value as the cooling progressed. After the temperature reached equilibrium, the volume relaxation caused the stresses to relax.
Comparing the transient thermal stresses and the birefringence, it can be noted that the birefringence sign also changes during the quenching, but not at the same time as the stresses. The stresses changed from tension at the surface to compression in matter of 1 s, while the birefringence changed gradually after this time. This is because the birefringence depends on the thermo-mechanical history that the polymer, at each point along the radius, experiences during the quenching. This means that when the stresses changed from tension (positive) to compression (negative), the birefringence was still influenced by the stress history and the birefringence sign did not change right after the stresses sign changed. Furthermore, in the case of PS, the time-temperature dependent strain-optical coefficient changed from negative to positive when the temperature decreased [11].

Fig. 7-9 shows the simulated transient thermal stresses for PC tube quenched in water from 180 to 25 °C.
Figure 7-9 Simulated transient thermal stresses for quenching PC tube from 180 to 25 °C: a) $\sigma_{rr}$, b) $\sigma_{\theta\theta}$, and c) $\sigma_{zz}$.

The simulated stresses in PC tubes developed in the same fashion as those in PS tubes (Fig 7-6). Nevertheless, the magnitude of the residual stresses (at time of $2 \times 10^5$ s) was lower than that of PS samples. This was because the stress for PC tubes relaxed significantly, as observed in Fig. 7-9 at time of $2 \times 10^5$ s.

Fig. 7-10 shows the simulated transient thermal birefringence $\Delta n$ and $n_{rr} - n_{\theta\theta}$ of a PC tube quenched in water from 180 to 25 °C.
Figure 7-10 Simulated transient thermally-induced birefringence for a tube of PC quenched in water from 180 to 25 ºC.

At the beginning of the quenching process, the birefringence developed in PC tubes was positive near the outer wall, it diminished passing through zero to an extensive negative region towards the inner wall. As the cooling progressed, the stresses at the outer surface became compressive and those near the inner wall became tensile, as shown in Fig. 7-9. Therefore, the birefringence sign changed showing a negative minimum at the outer wall. Then it decreased passing through zero to a positive maximum near the inner wall.

Fig. 7-11 shows the simulated transient stress differences, $\sigma_{zz}-\sigma_{rr}$ (a) and $\sigma_{rr}-\sigma_{\theta\theta}$ (b), for a PC tube quenched from an initial temperature of 180 ºC to 25 ºC. At the early stages of the quenching process (0.35 s), $\sigma_{zz}-\sigma_{rr}$ was positive at the outer wall and negative towards the center. As the cooling progresses, $\sigma_{zz}-\sigma_{rr}$ changed from positive to negative at the surface.
Figure 7-11 Simulated normal stress difference (a) $\sigma_{zz} - \sigma_{rr}$ and (b) $\sigma_{rr} - \sigma_{\theta\theta}$ for a PC tube quenched in water from 120 to 25 °C.

Simulations showed that the thermal stress difference of PS and PC developed in the same fashion during the quenching. However, the magnitude of the stress difference for PS were higher than that of the PC samples. Furthermore, the stress difference for the PC relaxed more than that of the PS tubes. This is a consequence of the high stress relaxation of the PC.

7.5 Thermally-Induced Residual Stresses and Birefringence in Polystyrene Tubes

Figs. 7-12 and 7-13 show, respectively, the measured and simulated thermally-induced birefringence components, $\Delta n$ and $n_{rr} - n_{\theta\theta}$, and the simulated residual stresses for a PS tube quenched in water from 105 to 25 °C. For this condition, the measured residual birefringence, $\Delta n$, was positive while the measured birefringence, $n_{rr} - n_{\theta\theta}$, was negative along the tube wall thickness. Simulations for this condition showed that, $\Delta n$ has a
positive maximum near the outer wall, then, it decreases passing through zero about \( r/R=0.75 \) to a negative value showing a minimum near the inner wall.

Figure 7-12 Measured (symbols) and simulated (lines) thermally-induced residual birefringence \( \Delta n \) and \( n_{rr}-n_{\theta\theta} \) for a PS tube quenched in water from 105 to 25 °C.

Figure 7-13 Simulated thermally-induced residual stresses in radial (\( \sigma_{rr} \)), circumferential (\( \sigma_{\theta\theta} \)) and axial (\( \sigma_{zz} \)) directions for a PS tube quenched in water from 105 to 25 °C.
The simulated thermally-induced residual stress distribution in the radial direction \( \sigma_{rr} \) was positive (tensile) through the wall thickness of the tube. It showed a zero magnitude at the inner and outer surfaces as required by the traction-free boundary condition imposed at the inner and outer walls of the tube. The circumferential and axial stress components, \( \sigma_{\theta \theta} \) and \( \sigma_{zz} \), had their largest magnitude at the inner and outer tube walls. Both components exhibited a positive maximum at the inner wall, then, they decreased passing through zero to a negative value, showing a negative minimum at the outer wall. Both stresses showed a parabolic-like distribution and the location of the zero value of axial stresses shifted towards the outer wall because of the equilibrium of the axial forces.

Figs. 7-14 and 7-15 show, respectively, the measured and simulated birefringence components, \( \Delta n \) and \( n_{rr} - n_{\theta \theta} \), and the simulated residual stresses with respect to the radius of a PS tube quenched in water from 120 to 25 °C. The measured birefringence components \( \Delta n \) and \( n_{rr} - n_{\theta \theta} \) showed a positive maximum near the outer wall, then, both components decreased passing through zero to a negative value, showing a highest negative value near the inner wall. The measured \( \Delta n \) and \( n_{rr} - n_{\theta \theta} \) were found to be of the same order of magnitude at the inner and outer walls of the tube. Furthermore, their distribution along the radius exhibited only small differences. Simulated \( \Delta n \) and \( n_{rr} - n_{\theta \theta} \) showed a positive maximum of near the outer wall, then it decreased passing through zero to a negative value showing a highest negative value near the inner wall.
Fig. 7-14 Measured (symbols) and simulated (lines) thermally-induced residual birefringence $\Delta n$ and $n_{\theta\theta}-n_{rr}$ for a PS tube quenched in water from 120 to 25 ºC.

Figure 7-15 Simulated thermally-induced residual stresses in radial ($\sigma_{rr}$), circumferential ($\sigma_{\theta\theta}$) and axial ($\sigma_{zz}$) directions for a PS tube quenched in water from 120 to 25 ºC.
Figs. 7-16 and 7-17 show, respectively, the measured and simulated thermally-induced residual birefringence components, $\Delta n$ and $n_{rr}-n_{\theta\theta}$, and the simulated residual stresses with respect to the radius for a tube of PS quenched from 135 to 25 °C. The measured $\Delta n$ and $n_{rr}-n_{\theta\theta}$ were positive near the outer wall, both birefringence components decreased passing through zero to negative values in an extensive region toward the inner wall. It is observed that at the initial temperature of 135 °C, the simulated birefringence was in good agreement with the measured one. It also showed a highest positive value at the outer wall, it decrease passing through zero to a highest negative value at the inner wall. Comparing Figs. 7-12, 7-14, and 7-16, it is observed that the magnitude of both components of the birefringence increased with the initial quenching temperature.

Fig. 7-16 Measured (symbols) and simulated (lines) thermally-induced residual birefringence $\Delta n$ and $n_{rr}-n_{\theta\theta}$ for PS tube quenched in 25 °C water from an initial temperature of 135 °C.
Figure 7-17 Simulated thermally-induced residual stresses in radial ($\sigma_{rr}$), circumferential ($\sigma_{\theta\theta}$) and axial ($\sigma_{zz}$) directions for a tube of polystyrene quenched from 135 to 25 °C.

It is important to note, in Figs. 7-14 and 7-16, that the positive and negative regions of the measured and simulated birefringence components of $\Delta n$ and $n_{rr} - n_{\theta\theta}$ are not balanced through the tube wall thickness, in the sense that integrals of the positive and negative parts are not equal to one another, i.e. $\int_0^R (n_r - n_{\theta}) \, dr \neq 0$. However, the positive and negative portions of the simulated residual stresses profile are balanced, as required by the equilibrium condition in the axial direction (Eq. 4-22). The unbalance distribution of the birefringence was due to the fact that the strain-optical coefficient is a function of time and temperature and the final birefringence is the result of the thermo-mechanical history that the polymer experienced during cooling [130,160].

Simulations showed that for the three initial temperatures, the residual stresses for free quenched viscoelastic tubes were tensile (positive) near the inner wall and compressive (negative) near the outer wall. The stresses increased when the initial
quenching temperature increased. However, at the initial temperature of 135 ºC the difference between the simulated residual stresses with respect to that at the initial temperature of 120 ºC was less than that observed between the initial temperatures of 105 and 120 ºC. Comparing the measured birefringence components, \( \Delta n \) and \( n_{rr} - n_{\theta\theta} \), quenched at initial temperatures of 120 and 135 ºC, it was noted that when the initial temperature increased, the radial location of the zero value of the birefringence shifted towards the outer tube wall.

7.6 Thermally-Induced Residual Stresses and Birefringence in Polystyrene Rods

Figs. 7-18 and 7-19 show, respectively, the measured and simulated birefringence \( \Delta n \) and \( n_{rr} - n_{\theta\theta} \) and the simulated residual stresses along the radius for a PS rod quenched from 105 to 25 ºC. The measured birefringence \( \Delta n \) showed a positive value along the radius of the rod. The measured birefringence \( n_{rr} - n_{\theta\theta} \) showed a positive magnitude near the surface of the rod, it decreased passing through zero to a negative region at the core of the rod. Simulated \( \Delta n \) showed a maximum near the surface of the rod, it decreased passing through zero to a negative region at the core of the rod. The simulated birefringence \( n_{rr} - n_{\theta\theta} \) showed a negative value near the surface of the rod. Then it passed through zero to a positive region. Then, it decreased passing once more through zero to a negative region in the core of the rod. It is important to mention that the thickness of the slices to measure the birefringence \( n_{rr} - n_{\theta\theta} \) had to be increased to 5 mm. However, the slice to measure \( \Delta n \) was 2 mm, since the thickness of the slice in the plane \( z-r \) (Fig. 5-6) could not be increased due to the cylindrical cross-sectional area of the rod. The positive value of \( \Delta n \) could have been caused due to a distortion of the birefringence.
Figure 7-18 Measured (symbols) and simulated (lines) birefringence $\Delta n$ and $n_{\theta\theta} - n_{rr}$ for a polystyrene rod quenched in water from 105 to 25 °C.

Figure 7-19 Simulated thermal stresses in radial ($\sigma_{rr}$), circumferential ($\sigma_{\theta\theta}$) and axial ($\sigma_{zz}$) direction for a polystyrene rod quenched in water from 105 to 25 °C.
profile when the sample was cut. This hypothesis was proved to be correct when the birefringence $n_{rr} - n_{\theta\theta}$ was measured in slices of different thicknesses. Fig. 7-20 shows the measured birefringence $n_{rr} - n_{\theta\theta}$ for a rod quenched from 105 to 25 °C at two different slice thickness, 2 and 5 mm.

![Figure 7-20](image_url)

Figure 7-20 Measured birefringence $n_{rr} - n_{\theta\theta}$ for a rod of PS quenched from 105 to 25 °C at two different slice thickness, 2 and 5 mm.

For a 2 mm slice thickness, the birefringence $n_{rr} - n_{\theta\theta}$ was positive throughout the radius. When the thickness of the slice was increased to 5 mm, $n_{rr} - n_{\theta\theta}$ showed a positive value near the surface, it decreased passing through zero to a negative value at the center. The distortion of the birefringence at low initial quenching temperature (i.e. 105 °C) and at low slice thickness can be attributed to thermally-induced stresses in the elastic range, since the initial temperature was very close to $T_g$. Therefore, the molecules are frozen and the long-range molecular motions are hindered [161]. This could lead to a segmental orientation and bond deformation [162, 163], in turn causing changes in birefringence.
when the thin slice was removed from the sample. However the question remains open and further investigation will be needed in order to understand this effect.

Simulated radial, circumferential, and axial stresses exhibited a positive maximum at the rod core. The radial stress decreased along the radius and vanishes at the rod surface, as required by the traction-free boundary condition. The circumferential and axial stresses decreased along the radius passing through zero to a negative value (compressive stresses), showing a highest negative value at the rod surface. The radial and circumferential stresses at the rod center were equal and lower than the axial stress value at the center. The stress $\sigma_{zz}$ was in equilibrium, in the sense that the positive and negative forces were equal to each other i. e. $2\pi\int_0^2 \sigma_{zz} r dr = 0$.

Figs. 7-21 and 7-22 show, respectively, the measured and simulated birefringence $\Delta n$ and $n_{rr}-n_{\theta\theta}$ and the simulated residual stresses for PS rod quenched in water from 120 to 25 °C. The birefringence $\Delta n$ was higher near the wall and near the core region than the birefringence $n_{rr}-n_{\theta\theta}$. $\Delta n$ showed a positive maximum near the outer wall and decreased passing through zero to a negative value. It is important to note that the birefringence $n_{rr}-n_{\theta\theta}$ had a zero magnitude at the center. This is because, the plane strain approximation (employed in the present simulations) makes the radial and circumferential strains ($\varepsilon_{rr}$ and $\varepsilon_{\theta\theta}$) equal at the center of the rod ($r=0$). This is evident from equations 4-19 and 4-20 shown in Chapter IV. Combining these two equations yields $\varepsilon_{\omega\omega} = \frac{1}{r} \int_0^r \varepsilon_{zz} dr$. Using the L’Hospital rule, this equation leads to $\varepsilon_{\omega\omega} = \varepsilon_{zz}$ when the $r=0$. To avoid this problem, the strains should be calculated using a three-dimensional approach where the strain $\varepsilon_{zz}$
would not be constant along the radius as assumed in the plane strain approximation (employed in the present simulations).

![Diagram showing birefringence and thermal stress](image)

**Figure 7-21** Measured (symbols) and simulated (lines) birefringence $\Delta n$ and $n_{rr}-n_{\theta\theta}$ for a PS rod quenched in water from 120 to 25 °C.

![Diagram showing thermal stresses](image)

**Figure 7-22** Simulated thermal stresses in radial ($\sigma_{rr}$), circumferential ($\sigma_{\theta\theta}$) and axial ($\sigma_{zz}$) direction for a PS rod quenched in water from 120 to 25 °C.
The simulated residual stresses in rods quenched from 120 °C to 25 °C, developed in the same fashion as those developed for an initial temperature of 105 °C. However, their magnitude increased with the initial temperature. With further increase of the initial temperature, the relative increase of thermally-induced residual stresses reduced, since the stress relaxation increases with temperature.

Figs. 7-23 and 7-24 show, respectively, the measured and simulated thermally-induced residual birefringence, $\Delta n$ and $n_{rr} - n_{\theta\theta}$, and simulated residual stress components for a PS rod quenched from 135 °C to 25 °C. The measured $\Delta n$ showed a highest positive value near the outer wall. It decreased passing through zero to a negative value in the core. When the initial temperature increased, the location where the birefringence $\Delta n$ and $n_{rr} - n_{\theta\theta}$ change from positive to negative, shifted towards the outer wall. Simulations showed that the increase of residual stresses was less when the initial temperature increased from 120 to 135 °C compared to the increase observed between the initial temperatures of 105 and 120 °C. This is because when the temperature increased, the stress relaxation was faster and the contribution of the stresses at high temperature became less. Furthermore, it has been reported that the residual stresses are nearly independent of initial temperature when it is much above $T_g$ [158].

The simulated thermally-induced residual stresses at the three temperatures were found to be always positive in the core and negative at the surface. The stress distribution in axial direction, $\sigma_{zz}$, showed a parabolic shape. It exhibited a highest compressive stress at the surface and highest tensile stress at the core. The parabolic distribution of thermally-induced residual stresses has been observed in free quenched experiments performed on flat plates of polymer [124] and inorganic glass [139].
Figure 7-23 Measured and simulated birefringence $\Delta n$ and $n_{rr}-n_{\theta\theta}$ for a polystyrene rod quenched in water from 135 to 25 °C.

Figure 7-24 Simulated thermally-induce residual stresses in radial ($\sigma_{rr}$), circumferential ($\sigma_{\theta\theta}$) and axial ($\sigma_{zz}$) directions for a polystyrene rod quenched in water from 135 to 25 °C.

To avoid the influence of the heat transfer on the birefringence at the ends of the tubes and rods, the average birefringence, $<n_{zz}-n_{\theta\theta}>$, was measured at the center of the length of the rod. Fig. 7-25 shows the average birefringence with respect to the length of
a PS rod quenched from 135 to 25 °C. It was observed that the average birefringence from the center of the rod up to 5 mm before the end remained almost constant. However, near the end of the rod, the birefringence passed through a minimum. Then, it increased to a highest value near the end of the rod.

Figure 7-25 Measured average birefringence $\langle n_{zz}-n_{\theta\theta} \rangle$ with respect to the distance from the middle of a PS rod free-quenched from an initial temperature of 135 to 25 °C.

The variation of the average birefringence near the end of the rod was due to the heat removal from the ends of the rod that led to a different stress distribution than that at the center of the length of the rod.

Fig. 7-26 shows the measured and simulated average birefringence, $\langle n_{zz}-n_{\theta\theta} \rangle$ for free-quenched tubes and rods of PS at different initial temperatures. It was observed that the average birefringence for both the tube and the rod quenched from an initial temperature of 105 °C was positive. The average birefringence of the tubes quenched from 120 and 135 °C became negative and exhibited a low magnitude.
Figure 7-26 Measured (symbols) and simulated (lines) average birefringence in PS tubes and rods.

The average birefringence for the rods quenched from 120 and 135 °C also became negative and its magnitude increased with temperature. Simulated average birefringence at low initial temperature (105 °C) showed large discrepancies from measurements. It was observed that the average birefringence for an initial temperature for both tubes and rods were negative and its magnitude was very low. When the initial temperature increased, the value of the simulated average birefringence, which is negative for tubes, slightly increased. For the rods, the magnitude of the average birefringence also increased with temperature. Furthermore, the average birefringence of the rods quenched from 120 and 135 °C was higher than the average birefringence of tubes quenched at the same temperature. The simulated average birefringence for rods exhibited large discrepancies with experiments. The positive value of the measured average birefringence could be
attributed to the positive strain-optical coefficient observed in PS at temperatures below \( T_g \), caused by the orientation of the phenyl group [102]. For an initial temperature of 105 °C, the sample cooled faster below \( T_g \). Therefore, the thermal stresses generated a positive birefringence. Simulations could not describe this phenomenon.

7.7 Thermally-Induced Residual Stresses and Birefringence in Polycarbonate

Figs. 7-27 and 7-28 show, respectively, the measured and simulated birefringence components, \( \Delta n \) and \( n_{rr}-n_{\theta\theta} \), and the simulated residual stresses along the radius of a polycarbonate tube quenched in water from 170 to 25 °C. Near the outer wall, both birefringence components \( \Delta n \) and \( n_{rr}-n_{\theta\theta} \) show a negative minimum. Then, their magnitude increases passing through zero to a positive region near the inner wall. The magnitude of the measured \( \Delta n \) at the outer and inner tube walls was lower than that of \( n_{rr}-n_{\theta\theta} \). Furthermore, the location where \( \Delta n \) changed from negative to positive value (zero magnitude) shifted towards the outer wall with respect to that of \( n_{rr}-n_{\theta\theta} \). It is important to note in Fig. 7-27 that the measured \( \Delta n \) showed a maximum and then decreased towards the inner wall. This effect could have been caused by a redistribution of stresses when the sample was cut in the plane \( z-r \). This effect was not observed in the birefringence \( n_{rr}-n_{\theta\theta} \). The simulated components of birefringence \( \Delta n \) and \( n_{rr}-n_{\theta\theta} \) showed a negative maximum near the outer wall, then it decreased passing through zero to a positive value reaching a highest value at the inner wall. The simulated circumferential and axial residual stresses for a PC tube also showed a highest positive value at the inner wall (Fig. 7-28). The simulated radial stresses are tensile throughout the radius and vanish at the inner and outer surfaces. The simulated residual stresses in PC tubes were lower than the residual
stresses in PS tubes. This was because the stress relaxation of the PC was more significant than the stress relaxation of PS since the relaxation time, $\theta_r$ (Eq. 4-6), for PC was larger than that of PS.

![Figure 7-27](image1.png)

**Figure 7-27** Measured (symbols) and simulated (lines) Thermally-induced residual birefringence for a polycarbonate tube quenched in water from 170 to 25 °C.

![Figure 7-28](image2.png)

**Figure 7-28** Simulated thermally-induced residual stresses in radial ($\sigma_{rr}$), circumferential ($\sigma_{\theta\theta}$) and axial ($\sigma_{zz}$) direction for a polycarbonate tube quenched in water from 170 to 25 °C.
Figs. 7-29 and 7-30 show, respectively, the measured and simulated birefringence components, $\Delta n$ and $n_{rr}-n_{\theta\theta}$, and the simulated stress components along the radius for a polycarbonate tube quenched from 180 to 25 ºC. For an initial temperature of 180 ºC the measured birefringence $\Delta n$ increased slightly near the outer wall with respect to the measured $\Delta n$ at 170 ºC. Furthermore, the location where the birefringence change from negative to positive (zero magnitude), shifted slightly towards the outer wall. The birefringence $\Delta n$ near the inner wall increased with the initial temperature. The measured birefringence $n_{rr}-n_{\theta\theta}$ increased slightly near the outer wall, the location where the birefringence change from negative to positive value shifted towards the outer wall. Near the inner wall, $n_{rr}-n_{\theta\theta}$, increased when the initial temperature increased from 170 to 180 ºC.

![Normalized radius (r/R) vs. Birefringence (x10^-3)](image)

Figure 7-29 Measured (symbols) and simulated (lines) thermally-induced residual birefringence for polycarbonate tube quenched from 180 to 25 ºC.
Figure 7-30 Simulated thermally-induced residual stresses in radial ($\sigma_{rr}$), circumferential ($\sigma_{\theta\theta}$) and axial ($\sigma_{zz}$) direction for a polycarbonate tube quenched in water from 180 to 25 °C.

The simulated axial and circumferential residual stresses were tensile near the inner wall and compressive near the outer wall. The radial stresses were tensile through the wall thickness and zero at both surfaces. The residual stresses in quenched tubes of polycarbonate behaved in the same fashion as those for polystyrene tubes. However, the magnitude of the thermally-induced residual stresses was lower. It was observed that, in general, the value of the simulated residual stresses for PC tubes were lower than the simulated residual stresses for PS tubes. This was because the stresses relaxation in PC samples was higher than the stress relaxation of the PS samples as observed in Fig. 7-6 and Fig. 7-9.
7.8 Thermally-Induced Residual Stresses and Birefringence in Polycarbonate Rods

Figs. 7-31 and 7-32 show, respectively, the measured and simulated birefringence components, $\Delta n$ and $n_{rr}-n_{\theta\theta}$, and the simulated thermally-induced residual stresses along the radius of a PC rod quenched from 170 to 25 °C. At the outer wall, the measured $\Delta n$ was higher than the measured $n_{rr}-n_{\theta\theta}$. At the center, their magnitudes were similar. Also, the location where the measured $\Delta n$ changed its sign was closer to the rod surface than the location where the measured $n_{rr}-n_{\theta\theta}$ changed its sign. The magnitude of the simulated $\Delta n$ was higher at the surface than that of the simulated $n_{rr}-n_{\theta\theta}$. The location where the simulated $\Delta n$ changed its sign was closer to the surface than the location where the simulated $n_{rr}-n_{\theta\theta}$ changed its sign.

![Figure 7-31](image)

Figure 7-31 Measured (symbols) and simulated (lines) thermally-induced residual birefringence for polycarbonate rod quenched from 170 to 25 °C.
Figure 7-32 Simulated thermally-induced residual stresses in radial ($\sigma_{rr}$), circumferential ($\sigma_{\theta\theta}$) and axial ($\sigma_{zz}$) direction for a polycarbonate rod quenched in water from 170 to 25 °C.

Figs. 7-33 and 7-34 show, respectively, the measured and simulated birefringence components, $\Delta n$ and $n_{rr} - n_{\theta\theta}$, along the radius of a PC rod quenched in water from 180 to 25 °C.

Figure 7-33 Measured (symbols) and simulated (lines) thermally-induced residual birefringence for polycarbonate rod quenched from 180 to 25 °C.
The measured $\Delta n$ is higher at the wall than the measured $n_{rr}-n_{\theta \theta}$. Also, the magnitude of the measured $\Delta n$ was higher at the center than the measured $n_{rr}-n_{\theta \theta}$.

Figure 7-34 Simulated thermally-induced residual stresses in radial ($\sigma_{rr}$), circumferential ($\sigma_{\theta \theta}$) and axial ($\sigma_{zz}$) direction for a polycarbonate tube quenched in water from 180 to 25°C.

Fig. 7-35 shows the measured and simulated average birefringence $<n_{zz}-n_{\theta \theta}>$ for PC tubes and rods. In general, the average birefringence for rods was higher than the average birefringence of tubes. The average birefringence increased when the initial temperature increased. The simulated average birefringence for both, the tubes and the rods was lower than the measured birefringence for the two initial temperatures employed.
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Initial temperature (°C)

165 170 175 180 185

Birefringence \( \Delta n_{\text{avg}} \) (x10^4)

0.0 1.0 2.0 3.0 4.0 5.0

Measured (tube)

Measured (rod)

Simulated (tube)

Simulated (rod)

Figure 7-35 Measured (symbols) and simulated (lines) average birefringence of PC and tubes and rods.

7.9 Influence of the Wall Thickness of Tube on the Simulated Thermally-Induced Stresses and Birefringence.

Fig. 7-36 shows the influence of the wall thickness on the simulated thermally-induced residual stresses in radial (a), circumferential (b), and axial (c) directions and The thermally-induced residual stresses increased when the wall thickness increased. Furthermore, the magnitude of the birefringence increased with the thickness of the wall.
Figure 7-36 Simulated radial, $\sigma_{rr}$ (a), circumferential, $\sigma_{\theta\theta}$ (b), and axial, $\sigma_{zz}$ (c), thermal stresses for a PS tube quenched from 135 to 25 °C, with different wall thicknesses.

Fig 7-37 shows the simulated birefringence $\Delta n$ (a), $n_{rr}-n_{\theta\theta}$ (b) and average birefringence $<n_{zz}-n_{\theta\theta}>$ (c). Simulations showed that the birefringence $\Delta n$ and $n_{rr}-n_{\theta\theta}$ increases with the wall thickness. The absolute magnitude of the simulated average birefringence, $<n_{zz}-n_{\theta\theta}>$, increased with the wall thickness.
Figure 7-37 Simulated birefringence $\Delta n$ (a), $n_r-n_\theta$ (b), and average birefringence $\langle n_{zz}-n_\theta \rangle$ (c) for a PS tube quenched from 135 to 25°C, with different wall thicknesses.

7.10 Conclusions

Thermally-induced residual stresses and birefringence were measured and simulated in tubes and rods of PS and PC. In general, the magnitude of thermally-induced birefringence of free-quenched tubes and rods of PC was higher than that for PS samples. This was because the strain-optical coefficient of PC was higher than that of the PS near
the glass transition temperature. However, the magnitude of the simulated residual stresses for tubes and rods of PS was higher than that for the corresponding PC samples. This was because the stress relaxation of the PC was more significant than the stress relaxation of PS since the relaxation time, $\theta_r$ (Eq. 4-6), for PC was larger than that of PS.

For an ideal elastic tube, the analytical and numerical solutions of the thermal stresses were comparable to one another and the results did not show numerical instabilities. However, for viscoelastic tubes and rods, the simulated stresses and birefringence showed numerical instabilities, especially near the outer wall where the cooling proceeds faster than at the inner wall (tubes) and core (tubes). The instabilities occurred because the modulus of the polymer changed significantly when the temperature drops from above to below $T_g$. This caused that the derivatives of $C_1$, $C_2$, and $C_3$ in Eq. 4-42 which are functions of the modulus (Eqs. 4-34, 4-35, and 4-36) became large leading to numerical instabilities. However, it was found that increasing the number of meshes in the radial direction, the magnitude of residual stresses converged to a steady value. Simulations also showed that the residual stresses and birefringence increased when the wall thickness of the tube increased.

The tubes and rods of PS were quenched at low initial temperature (105 °C). The measured birefringence $n_{rr} - n_{\theta\theta}$ was positive throughout the radius when the thickness of the sample was 2 mm. However, for the rods of PS, by increasing the thickness of the slices from 2 to 5 mm, the birefringence showed a positive value near the outer wall and a negative value at the core. The birefringence $\Delta n$ for the tubes and rods quenched at 105 °C was positive throughout the radius. The thickness of the slices employed to measure the birefringence $\Delta n$ in PS samples could not be increased beyond 2 mm because the
color sequence in the compensator became unclear. This is due to the circular geometry of the samples, since by increasing the thickness of the slice in the plane $z-r$ (Fig. 5-6), the light traveling in the $\theta$ direction would pass through different radial positions (see Fig. 5-6). At this initial quenching temperature, simulated birefringence showed a large deviation from the measured birefringence. This could be attributed to thermally-induced stresses in the elastic range, since the initial temperature of 105 °C was very close to $T_g$. Therefore, during quenching, the molecules were quickly frozen and the long-range molecular motion was hindered. This could lead to a segmental orientation and bond deformation, in turn causing changes in birefringence when the slice was removed from the sample. However, the question remains open and further investigation will be needed in order to understand this effect. When the initial quenching temperature of the PS samples was increased, the simulated birefringence showed a better agreement with experiments. This can be attributed to the increase of molecular mobility at a high initial quenching temperature. This could have led to an increase of the long-range molecular orientation that remained after the slice was removed from the quenched sample.

The measured birefringence $n_{rr} - n_{\theta\theta}$ showed a plateau at the core of the PS and PC rods. However, simulated birefringence $n_{rr} - n_{\theta\theta}$ showed a zero magnitude at the center of the rods of PS and PC. This was because, by using the plane-strain approximation to calculate the thermally-induced stresses, in the radial ($\sigma_{rr}$) and circumferential ($\sigma_{\theta\theta}$) directions were equal at the center of the rod in the plane $r-\theta$. As a consequence, at this location, the refractive indices were equal in the radial and circumferential directions rendering a zero magnitude of birefringence.
The birefringence $\Delta n$ for the tubes and rods of PC showed a negative value near the outer wall and a positive near the inner wall (for tubes) and core (for rods). The magnitude of the birefringence increased with the initial quenching temperature and the location where the birefringence change from negative to positive shifted towards the outer wall when the initial quenching temperature increased.

The average birefringence in tubes and rods of PS quenched at 105 °C was positive. The simulated average birefringence at an initial temperature of 105 °C has negative value for both tubes and rods. This discrepancy was attributed to the positive strain optical coefficient of PS at temperatures below $T_g$, caused by the orientation of the phenyl group. This effect could not be described by the present model. When the initial quenching temperature increased, both the measured and simulated average birefringences were negative. The measured and simulated average birefringence for tubes and rods of PC were positive and increased with the initial quenching temperature.
CHAPTER VIII
TOTAL BIREFRINGENCE IN GAIM MOLDINGS

This chapter presents the measured and simulated total birefringence in GAIM moldings of PS and PC. The simulated total birefringence takes into account the contributions of both flow- and thermally-induced birefringence. Strictly speaking, the thermally-induced birefringence should be treated simultaneously with the flow-induced birefringence using a unique model and not by separate models, as indicated in Section 4.5. This is because, during the filling and gas-penetration stages, the melt experiences simultaneously large deformations due to flow, and small thermal contraction because of cooling. However, due to the lack of a unique model that can describe the stresses generated during the flow and thermal contraction at the same time, in the present simulations, flow-induced birefringence was calculated using a non-linear model and thermally-induced birefringence components were calculated using a linear viscoelastic model based on the temperature history that the polymer experienced during the GAIM cycle. As a first approximation, the coupled effect of flow and thermal deformations was not considered. Then, the thermally-induced birefringence, calculated according to the approach presented in Chapter IV, was added to corresponding flow-induced birefringence calculated, according to the procedure presented in Chapter III, using a non-linear model. The following sections show the effect of the processing conditions on the total birefringence distributions of $\Delta n$ and $n_{rr}-n_{\theta\theta}$ in GAIM moldings.
8.1 Contribution of Thermal Birefringence in PS GAIM Moldings

This section presents an example of how the thermally-induced birefringence (calculated according to the approach shown in Chapter IV) was added to the simulated flow-induced birefringence (presented in Chapter V) to obtain the total simulated birefringence in GAIM moldings.

Fig. 7-1 shows the measured and the individual components of the simulated flow- and thermally-induced birefringence, \( \Delta n \), for PS Run No. 2, at a melt temperature of 200 °C, at various distances from the sprue entrance: (a) and (b) in the sprue region at 4 and 6.5 cm, (c) and (d) in the primary gas penetration region of the spiral at 11 and 16 cm, and (e) in the solid region at 28 cm. As explained in Section 6.4, the birefringence, \( \Delta n \), near the outer wall was mainly caused by shear and normal stresses generated during the filling stage. In the case of PS moldings, simulations showed that the thermally-induced birefringence, \( \Delta n \), near the outer wall was one order of magnitude lower than the flow-induced birefringence. In this region, the flow-induced birefringence was negative while the thermally-induced birefringence was positive. However, near the inner wall, the magnitude of the flow-induced \( \Delta n \) was almost negligible. This is because, when the flow stopped, the flow-induced \( \Delta n \) relaxed near the inner wall of the GAIM molding, due to the high temperature of this region. However, simulations showed that the thermal contraction that occurred during cooling built-up the birefringence that was negligible near the inner wall. In the solid section, the measured \( \Delta n \) showed a maximum near the outer wall and an extensive plateau in the core region.
Figure 8-1 Measured (symbols) and simulated (lines) flow- and thermally-induced $\Delta n$ for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 2.
The simulated flow-induced $\Delta n$ relaxed almost completely in the core region. However, simulations showed that the thermal stresses generated during the cooling built-up the birefringence in the core region.

Fig. 8-2 shows the measured and simulated total birefringence, $\Delta n$, for PS Run No. 2 at different distances from the sprue entrance. When the thermally-induced $\Delta n$ was added to the corresponding flow-induced $\Delta n$, the simulated total birefringence provided a better qualitative description of the measured birefringence in PS GAIM moldings. Simulations showed that, for the case of PS, $\Delta n$ near the outer wall was caused mainly by flow, since the magnitude of the thermally-induced $\Delta n$ at this location was significantly lower than the corresponding flow-induced $\Delta n$. On the contrary, the birefringence near the inner wall was mostly caused by thermal stresses generated during cooling, since the flow-induced birefringence relaxed almost completely in this region when the flow stopped. In the solid region, the measured $\Delta n$ in the core was significantly lower than that near the outer wall. Simulated total $\Delta n$ showed that the birefringence in the core region of the solid section of the molding was caused by thermal stresses. Simulations also showed that for PS GAIM moldings, at all locations analyzed, the magnitude of the thermally-induced birefringence $\Delta n$ near the outer wall was very low, compared to the corresponding flow-induced birefringence. Therefore, the flow-induced $\Delta n$, near the outer wall was not significantly modified when the thermally-induced birefringence was added using the procedure explained in Section 4.5. However, the measured $\Delta n$ near the inner wall and that in the core region of the solid section, was only possible to describe by the simulated thermally-induced birefringence.
Figure 8-2 Measured (symbols) and simulated (lines) total birefringence, $\Delta n$, for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 2.
Fig. 8-3 shows the measured and the simulated flow- and thermally-induced
birefringence, $n_{rr} - n_{\theta\theta}$, for PS Run No. 2, at a melt temperature of 200 °C, at various
distances from the sprue entrance: (a) and (b) in the sprue region at 4 and 6.5 cm, (c) and
(d) in the primary gas penetration region of the spiral at 11 and 16 cm, and (e) in the solid
region at 28 cm. The measured $n_{rr} - n_{\theta\theta}$ showed a maximum near the outer wall, it showed
a minimum at the intermediate region and then increased towards the inner wall, showing
a maximum. The simulated flow-induced birefringence, $n_{rr} - n_{\theta\theta}$, showed a maximum near
the outer wall. However, near the inner wall, the flow-induced $n_{rr} - n_{\theta\theta}$, relaxed almost
completely, since the high temperature of this region allowed the stresses to relax when
the flow stopped. The simulated thermally-induced $n_{rr} - n_{\theta\theta}$ showed a negative value near
the outer wall, it increased, passing through zero to a positive value, showing a maximum
at the inner wall. Simulations showed that the flow- and thermally-induced $n_{rr} - n_{\theta\theta}$ near
the outer wall had a similar magnitude but opposite sign.

Fig. 8-4 shows the measured and simulated total birefringence, $n_{rr} - n_{\theta\theta}$, for PS Run
No. 2. The measured birefringence $n_{rr} - n_{\theta\theta}$ showed a maximum value at both the inner and
outer walls. However, simulated total $n_{rr} - n_{\theta\theta}$ showed a maximum at an intermediate
region caused by flow-induced birefringence. As stated in Section 6.4, the simulated
flow-induced $n_{rr} - n_{\theta\theta}$ was significantly lower than the simulated flow-induced $\Delta n$.
Therefore, the contribution of the thermally-induced $n_{rr} - n_{\theta\theta}$ was significant for this
birefringence component. It is important to note that, in the solid region at 28 cm from
the sprue entrance, the total simulated birefringence, $n_{rr} - n_{\theta\theta}$, showed a zero magnitude at
the center of the cylinder. This is because of the use of the plane strain approximation in
the thermal stress calculation, as explained in Section 7.6.
Figure 8-3 Measured (symbols) and simulated (lines) flow- and thermally-induced $n_{\theta\theta}$, for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 2.
Figure 8-4 Measured (symbols) and simulated (lines) total birefringence, $n_{rt}-n_{00}$, for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 2.
8.2 Total Birefringence in PS GAIM Moldings

The following sections present the influence of the processing conditions on the simulated total birefringence, $\Delta n$ and $n_{rr}-n_{\theta\theta}$, for PS GAIM moldings. The total birefringence comprises both the flow- and the thermally-induced birefringence added according to the procedure explained in Section 4.5 and illustrated in Section 8.1. The simulated results are compared with measurements previously shown in Chapter V.

8.2.1 The Effect of Melt Temperature on the Total Birefringence of PS GAIM Moldings

Figs. 8-5, 8-6, and 8-7 show the measured and the simulated total birefringence, $\Delta n$, for PS Runs No. 1, 2, and 3, at melt temperature of 180, 200 and 230 °C, respectively, at various distances from the sprue entrance: (a) and (b) in the sprue region at 4 and 6.5 cm, (c) and (d) in the primary gas penetration region of the spiral at 11 and 16 cm, and (e) in the solid region at 28 cm. Simulations and measurements showed that the maximum of $\Delta n$ near the outer wall decreased when the melt temperature increased. The simulated total $\Delta n$ near the inner wall showed that it decreased when the temperature increased.

This is the result of two combined effects. On one hand, the flow-induced birefringence decrease when the melt temperature increased. On the other hand, increasing the melt temperature the thermally-induced birefringence increased. However, at a temperature well above $T_g$ the stresses and birefringence relax very fast [102]. Therefore, above 180 °C, the contribution thermally-induced birefringence was minimal. On the other hand, the RWT decreased when the melt temperature increased, as discussed in Section 6.2.1. The reduction of the RWT leads to a lower thermally-induced birefringence at the inner wall, as shown in Section 7.9.

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Figure 8-5 Measured (symbols) and simulated (lines) total $\Delta n$, for a PS tubular GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 1 at melt temperature of 180 °C.
Figure 8-6 Measured (symbols) and simulated (lines) total birefringence, $\Delta n$, for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 2 at melt temperature of 200 °C.
Figure 8-7 Measured (symbols) and simulated (lines) total birefringence, $\Delta n$, for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 3 at melt temperature of 230°C.
The total birefringence decreased when the melt temperature increased mainly because the flow-induced birefringence decreased when the temperature increased.

Fig. 8-8 contrasts the effect of melt temperature on (a) measured and (b) simulated total birefringence, $\Delta n$, for PS Runs No. 1, 2, and 3 at melt temperatures of 180, 200, and 230 ºC, at 4 cm from the sprue entrance. It is evident that the measured $\Delta n$ near the outer wall decreased when the melt temperature increased. Furthermore, the thickness of the frozen-in birefringence decreased when the melt temperature increased. Simulations qualitatively agreed with measurements. However, the predicted birefringence was higher than the simulated one. The deviation between measurements and simulations may have been due to cooling.

Figure 8-8 Measured (a) and simulated (b) total birefringence $\Delta n$ for PS Runs No. 1, 2, and 3, at melt temperatures of 180, 200, and 230 C.

Figs. 8-9, 8-10, and 8-11 show the measured and the simulated total birefringence, $n_{rr} - n_{\theta\theta}$, for PS Runs No. 1, 2, and 3 at melt temperature of 180, 200 and 230 ºC, respectively.
Figure 8-9 Measured (symbols) and simulated (lines) total birefringence, \( n_{rr} - n_{\theta\theta} \), for a PS tubular GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 1 at melt temperature of 180 ºC.
Figure 8-10 Measured (symbols) and simulated (lines) total \( n_{rr} - n_{\theta\theta} \) for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 2 at melt temperature of 200 °C.
Figure 8-11 Measured (symbols) and simulated (lines) total $n_{tr}-n_{g,p}$ for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 3 at melt temperature of 230 ºC.
It is important to mention that, due to the low magnitude of the measured $n_{rr}-n_{\theta\theta}$ in PS moldings, no significant differences were observed among the three temperatures employed. It is also worth mentioning that the effect of the processing conditions on the birefringence $n_{rr}-n_{\theta\theta}$ in injection moldings was found to be minimal [2]. Simulations indicated that the total birefringence, $n_{rr}-n_{\theta\theta}$, at the outer wall decreased slightly when the temperature increased. This is chiefly due to the decrease of flow-induced birefringence when the melt temperature increased. Furthermore, it is important to mention that the birefringence $n_{rr}-n_{\theta\theta}$ at the center in the solid section of the spiral (Fig 5-7e, 5-8e, and 5-9e) showed a zero magnitude. This was because of the plane strain approximation employed to calculate the thermally-induced stresses, as explained in Section 6.5.

8.2.2 The Effect of Shot Size on the Total Birefringence of PS GAIM Moldings.

Figs. 8-12, 8-13, and 8-14 show the measured and the simulated total birefringence, $\Delta n$, for PS Runs No. 4, 5, and 6 at shot sizes of 75, 85, and 90%, respectively, at various distances from the sprue entrance: (a) and (b) in the sprue region at 4 and 6.5 cm, (c) and (d) in the primary gas penetration of the spiral at 11 and 16 cm, and (e) in the solid region. Simulations and measurements showed that, in the sprue region and primary gas penetration of the spiral, the shot size did not exert a strong influence on the total birefringence $\Delta n$. However, in the solid region, the simulated total $\Delta n$ showed a shoulder that decreased when the shot size increased. This shoulder was caused by the flow-induced birefringence, as discussed in Section 6.4.2. Simulations also showed that the thermally-induced $\Delta n$ increased slightly when the shot size decreased. This is because the gas-penetration time decreased slightly when the shot size decreased.
Figure 8-12 Measured (symbols) and simulated (lines) total birefringence, $\Delta n$, for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 45 cm, for Run No. 4 at shot size of 75%.
Figure 8-13 Measured (symbols) and simulated (lines) total birefringence, \( \Delta n \), for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 5 at shot size of 85%.
Figure 8-14 Measured (symbols) and simulated (lines) total birefringence, $\Delta n$, for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 6 at a shot size of 90%.

Therefore, the cooling proceeded faster in the region where the gas had cored-out the polymer. As a consequence, the thermally-induced birefringence increased.

Figure 8-15 contrasts the effect of shot size on measured (a) and simulated (b) total birefringence, $\Delta n$, for PS Runs No. 4, 5, and 6, at shot sizes of 75, 85, and 90%, at 4 cm from the sprue entrance. The maximum of the measured $\Delta n$ at the outer wall was
slightly lower for the shot size of 75%. However it is possible that this variation could have been due to experimental error. At the inner wall, the measured ∆n decreased slightly when the shot size increased.

Figure 8-15 Measured (a) and simulated (b) total birefringence ∆n for PS Runs No. 4, 5, and 6, at shot sizes of 75, 85, and 90%.

In spite of the increase of injection time with the shot size, simulations showed that there was almost no change of the thickness of the frozen-in layer of ∆n when the shot size increased.

Figs. 8-16, 8-17, and 8-18 show the measured and the simulated total birefringence, \( n_{rr} - n_{\theta\theta} \), for PS Runs No. 4, 5, and 6 at shot sizes of 75, 85, and 90%, respectively, at various distances from the sprue entrance: (a) and (b) in the sprue region at 4 and 6.5 cm, (c) and (d) in the primary gas penetration region of the spiral at 11 and 16 cm, and (e) in the solid region. Measurements and simulations showed that the shot size did not exert a strong influence on \( n_{rr} - n_{\theta\theta} \). However, simulations showed that the maximum of \( n_{rr} - n_{\theta\theta} \) located further away from the outer wall increased slightly with shot size.
Figure 8-16 Measured (symbols) and simulated (lines) total birefringence, $n_{tr}-n_{00}$, for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 45 cm, for Run No. 4 at a shot size of 75%.
Figure 8-17 Measured (symbols) and simulated (lines) total birefringence, $n_{rr} - n_{00}$, for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 5 at a shot size of 85%.
8.2.3 The Effect of Gas Pressure on the Total Birefringence of PS GAIM Moldings.

Figs. 8-19, 8-20, and 8-21 show the measured and the simulated total birefringence, $\Delta n$, for PS Runs No. 7, 8, and 9 at gas pressures 6.89 (1000), 10.34 (1500) and 13.79 (2000) MPa (psi), respectively, at various distances from the sprue entrance: (a) and (b) in the sprue region at 4 and 6.5 cm, (c) and (d) in the primary gas penetration of the spiral at 11 and 16 cm, and (e) in the solid region at 28 cm.
Figure 8-19 Measured (symbols) and simulated (lines) total birefringence, $\Delta n$, for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 7 at a gas pressure of 6.89 MPa.
Figure 8-20 Measured (symbols) and simulated (lines) total birefringence, \( \Delta n \), for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 8 at gas pressure of 10.34 MPa.
Figure 8-21 Measured (symbols) and simulated (lines) total birefringence, $\Delta n$, for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 9 at gas pressure 13.79 MPa.
For the gas pressure of 6.89 MPa (Fig. 8-19), the measured $\Delta n$ showed a small intermediate maximum around $r/R=0.8$ at all the locations in the primary gas penetration (sprue and primary gas penetration region of the spiral). For this condition, the simulated total birefringence, $\Delta n$, also showed a shoulder about $r/R=0.8$. However, its magnitude was higher than the measured one, as evident in Fig 8-19 d. Simulations also showed that this shoulder increases with the distance from the sprue entrance. For the gas pressures of 10.34 and 13.79 MPa, this shoulder was absent in the sprue region and primary gas penetration region of the spiral. However, in the solid section, at the location of 28 cm from the sprue entrance, simulated $\Delta n$ showed a shoulder that increased with gas pressure. Simulations showed that this shoulder was generated by the flow-induced stresses during the gas penetration stage, as discussed in Section 6.4.3.

Fig. 8-22 contrasts the effect of gas pressure on measured (a) and simulated (b) total birefringence, $\Delta n$, for PS Runs No. 7, 8, and 9 at gas pressures of 6.89, 10.34, and 13.79 MPa, at 4 cm from the sprue entrance. The maximum of the measured $\Delta n$ near the outer wall was similar for the three gas pressures employed since the processing variables during the filling stage were held constant. At the inner wall, the measured $\Delta n$ showed that its magnitude is comparable for the gas pressures of 10.34 and 13.79 MPa. However, for the gas pressure of 6.89 MPa, $\Delta n$ had the lowest magnitude. Near the inner wall, simulated $\Delta n$ increased slightly when the gas pressure increased. This is attributed to the increase of the flow-induced $\Delta n$ during the gas penetration, since increasing the gas pressure leads to higher flow-induced stresses and birefringence, as discussed in Section 6.2.3.
Figure 8-22 Measured (a) and simulated (b) total birefringence $\Delta n$ for PS Runs No. 7, 8, and 9, at gas pressures of 6.89, 10.34, and 13.79 MPa.

Figs. 8-23, 8-24, and 8-25 show the measured and the simulated total birefringence, $n_{rr} - n_{\theta\theta}$, for PS Runs No. 7, 8, and 9 at gas pressures of 6.89, 10.34 and 15.79 MPa, respectively, at various distances from the sprue entrance: (a) and (b) in the sprue region at 4 and 6.5 cm, (c) and (d) in the primary gas penetration region of the spiral at 11 and 16 cm, and (e) in the solid region at 28 cm. Measured birefringence, $n_{rr} - n_{\theta\theta}$, did not show significant differences between the three pressures employed. However, simulated $n_{rr} - n_{\theta\theta}$ showed a maximum that increased with the gas pressure. This is because low gas pressure leads to a higher relaxation of birefringence near the outer wall, as discussed in Section 6.2.3. The birefringence near the inner wall decreased when the gas pressure increased. This is because the RWT decreased when the gas pressure increased. As explained in Section 7.9, the thermally-induced birefringence decreases when the wall thickness decreased. As a consequence, the thermal stresses and birefringence were lower at the inner wall for the highest gas pressure since the RWT was thinner.
Figure 8-23 Measured (symbols) and simulated (lines) total birefringence $n_{rr}-n_{gh}$, for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm. For Run No. 7 at gas pressure 6.89 MPa.
Figure 8-24 Measured (symbols) and simulated (lines) total birefringence $n_{rr} - n_{o0}$ for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 8 at gas pressure of 10.34 MPa.
Figure 8-25 Measured (symbols) and simulated (lines) total birefringence \( n_{tr} - n_{00} \) for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 9 at gas pressure of 13.79 MPa.
8.2.4 The Effect of Injection Speed on Total Birefringence of PS GAIM Moldings

Figs. 8-26, 8-27, and 8-28 show the measured and the simulated total birefringence, $\Delta n$, for PS Runs No. 10, 11, and 12 at injection speed of 1.27, 7.62, and 15.24 cm/s, respectively, at various distances from the sprue entrance: (a) and (b) in the sprue region at 4 and 6.5 cm, (c) and (d) in the primary gas penetration region of the spiral at 11 and 16 cm, and (e) in the solid region. Simulations and experiments showed that the maximum of $\Delta n$ near the outer wall increased with the injection speed. This is because, as discussed previously in Section 6.2.4, by increasing the injection speed, the shear and normal stresses increased during the filling stage. As a consequence, the flow-induced birefringence increased. Furthermore, the thickness of the frozen-in $\Delta n$ near the outer wall decreased significantly when the injection speed increased, since high injection speed leads to a low filling time and thinner frozen layer. The simulated thermally-induced birefringence showed that the magnitude of $\Delta n$ increased slightly when the injection speed decreased. This is mainly due to the increase of the RWT when the injection speed decreased.

In the solid section, at 28 cm from the sprue entrance, the measured $\Delta n$ in the core region showed an extensive plateau for the three injection speeds employed. The $\Delta n$ magnitude of this plateau was lower than the magnitude of $\Delta n$ near the outer wall. Simulations showed that this plateaus were caused by thermal stresses generated during cooling. Simulations of $\Delta n$ at different injection speeds showed clearly that the birefringence near the outer wall of the PS molding was caused mainly by the flow-induced stresses generated during the filling stage and the birefringence near the inner wall was caused mainly by the thermally-induced stresses generated during cooling.
Figure 8-26 Measured (symbols) and simulated (lines) total $\Delta n$, for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 34 cm. For Run No. 10 at injection speed of 1.27 cm/s.
Figure 8-27 Measured (symbols) and simulated (lines) total $\Delta n$ for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm. For Run No. 11 at injection speed of 7.62 cm/s.
Figure 8-28 Measured (symbols) and simulated (lines) total $\Delta n$ for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 12 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 12 at an injection speed of 15.24 cm/s.
Figure 8-29 contrasts the effect of injection speed on the measured (a) and simulated (b) total birefringence, $\Delta n$, for PS Runs No. 10, 11, and 12 at injection speeds of 1.27, 7.62, and 15.24 cm/s, at 4 cm from the sprue entrance. Simulated results qualitatively described the effect of the injection speed on the birefringence, $\Delta n$. However, near the outer wall, the simulated $\Delta n$ was higher than the measured one for the three injection speeds employed. Near the inner wall at the lowest injection speed (1.27 cm/s), the simulated $\Delta n$ was slightly higher than that at higher injection speeds. This was caused by an increase of the thermally-induced $\Delta n$ due to the increase of the RWT when the injection speed decreased, as discussed in Section 7.9.

Figure 8-29 measured (a) and simulated (b) total birefringence $\Delta n$ for Runs No. 10, 11, and 12, at injection speeds of 1.24, 7.62, and 15.24 cm/s.

Figs. 8-30, 8-31, and 8-32 show the measured and the simulated total birefringence, $n_{rr} - n_{\theta\theta}$, for PS Runs No. 10, 11, and 12 at injection speed of 1.27, 7.62, and 15.24 cm/s, respectively, at various distances from the sprue entrance: (a) and (b) in the sprue region at 4 and 6.5 cm, (c) and (d) in the primary gas penetration region of the spiral at 11 and 16 cm, and (e) in the solid region.
Figure 8-30 Measured (symbols) and simulated (lines) total $n_{rr} - n_{\theta\theta}$ for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm. For Run No. 10 at an injection speed of 2.54 cm/s.
Figure 8-31 Measured (symbols) and simulated (lines) total $n_{00} - n_{rr}$ for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 11 at an injection speed of 7.62 cm/s.
Figure 8-32 Measured (symbols) and simulated (lines) total $\Delta n$ for a PS tubular GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 12 at an injection speed of 15.24 cm/s.
Measured and simulated $n_{ir} - n_{i0}$ showed that its maximum at the outer wall increased slightly with the injection speed. This is due to the increase of the flow-induced birefringence with injection speed. Furthermore, the intermediate maximum increased and shifted towards the outer wall when the injection speed increased. This is because the flow-induced birefringence increased with the injection speed and the frozen layer was thinner at the higher injection speed.

8.2.5 The Effect of Gas-Delay Time on Total Birefringence on PS GAIM Moldings.

Figs. 8-33, 8-34, and 8-35 show the measured and the simulated total birefringence, $\Delta n$, for PS Runs No. 13, 14, and 15 at gas delay times of 0, 3, and 6 s, respectively, at various distances from the sprue entrance: (a) and (b) in the sprue region at 4 and 6.5 cm, (c) and (d) in the primary gas penetration region of the spiral at 11 and 16 cm, and (e) in the solid section. When no gas-delay time was employed to make the samples, the measured $\Delta n$ showed its highest value at the outer wall, then, it decreased showing a plateau towards the inner wall. However, when gas-delay time was employed, measured $\Delta n$ showed a maximum further away from the outer wall (around $r/R=0.75$). This maximum was more evident in the sprue region (Figs. 8-34 a and b) than in the primary gas penetration region of the spiral (8-34 c and d). The magnitude of this maximum increased and shifted towards the inner wall when the gas-delay time increased, as observed in Figs. 8-35 and 8-36 (a and b). Simulations showed that the maximum of $\Delta n$ further away from the wall increased with respect to the distance from the sprue entrance, as observed in Figs. 8-34 c and d.
Figure 8-33 Measured (symbols) and simulated (lines) total $\Delta n$ for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 13 at a gas-delay time of 0 s.
Figure 8-34 Measured (symbols) and simulated (lines) total $\Delta n$ for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 32 cm, for Run No. 14 at a gas-delay time of 3 s.
Figure 8-35 Measured (symbols) and simulated (lines) total $\Delta n$ for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 15 at gas-delay time of 6 s.

It is important to note that the maximum away from the outer wall of simulated $\Delta n$ at gas-delay time of 6 s, at the locations of 11 and 16 cm from the sprue entrance (Fig. 8-36 c and d) was lower than the maximum away from the outer wall of simulated $\Delta n$ at gas-delay of 3 s at the same locations. This is due to the lower gas penetration speed at
gas-delay time of 6 s, due to the high viscosity of the polymer caused by the temperature drop during the delay time.

Fig. 8-36 shows the influence of the gas-delay time on the total birefringence $\Delta n$ for PS Runs No. 13, 14 and 15 at gas-delay times of 0, 3, and 6 s, at 4 cm from the sprue entrance. The simulated total birefringence agreed qualitatively with measurements. Simulations demonstrated that the intermediate maximum of $\Delta n$ was developed during the gas penetration stage, as discussed in Section 6.4.5. Near the inner wall, the maximum of $\Delta n$ increased with the gas-delay time. This is because the RWT increased with gas-delay time. Therefore, the thermally-induced stresses and birefringence increased. Furthermore, the flow-induced birefringence during the gas penetration increased with gas-delay time, as discussed in Section 6.4.5.

![Figure 8-36 Measured (a) and simulated (b) total birefringence $\Delta n$ for PS Runs No. 13, 14, and 15, at gas-delay time of 0, 3, and 6 s at 4 cm from the sprue entrance.](image)

Figs. 8-37, 8-38, and 8-39 show the measured and the simulated total birefringence, $n_{rr} - n_{\theta\theta}$, for PS Runs No. 13, 14, and 15 at gas delay times of 0, 3, an 6 s, respectively, at various distances from the sprue entrance: (a) and (b) in the sprue region.
at 4 and 6.5 cm, (c) and (d) in the primary gas penetration region of the spiral at 11 and 16 cm, and (e) in the solid region. For the gas-delay time of 0 s, simulated total $n_{rr} - n_{\theta\theta}$ showed a maximum close to the outer wall, this maximum was formed during the filling stage. For the gas-delay times of 3 and 6 s (Figs. 8-38 and 8-39), the maximum of $n_{rr} - n_{\theta\theta}$ close to the wall decreased because of the birefringence relaxation during the delay time. However, during the gas penetration stage, the flow of the polymer created another maximum that shifted towards the inner wall when the gas delay-time increased. Furthermore, the value of this maximum increased when the gas-delay time increased. When the contribution of the thermally-induced $n_{rr} - n_{\theta\theta}$ was taken into account, the total simulated birefringence showed a higher value near the inner wall when the gas-delay time increased. This is because, the RWT increased with the gas-delay time, as discussed in Section 5.5.5. As a consequence, the contribution of the thermally-induced birefringence increased yielding a higher maximum of $n_{rr} - n_{\theta\theta}$ near the inner wall.
Figure 8-37 Measured (symbols) and simulated (lines) total $n_{\theta \theta} - n_{r r}$ for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 13 at a gas-delay time of 0 s.
Figure 8-38 Measured (symbols) and simulated (lines) total $n_{r \theta} - n_{\theta \theta}$ for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm. For Run No. 14 at a gas-delay time of 3 s.
8.2.6 The Effect of Mold Temperature on Total Birefringence of PS GAIM Moldings.

Figs. 8-40 and 8-41 show the measured and the simulated total birefringence, $\Delta n$, for PS Runs No. 16 and 17 at mold temperature of 30 and 60 °C, respectively, at various distances from the sprue entrance: (a) and (b) in the sprue region at 4 and 6.5 cm, (c) and
(d) in the primary gas penetration region of the spiral at 11 and 16 cm, and (e) in the solid region at 28 cm. The maximum of the measured $\Delta n$ at the outer wall did not show a significant change when the mold temperature was varied. However, the thickness of the frozen-in layer increased when the mold temperature decreased. This was caused by a faster cooling when the mold temperature reduced. In the solid region, the shoulder formed during the gas penetration was broader for the mold temperature of 30 °C than that for the mold temperature of 60 °C. This is because of the faster cooling at low mold temperature. Therefore, the flow-induced birefringence increased, especially near the outer wall, where the temperature gradient was higher.

Fig. 8-42 contrasts the effect of the mold temperature on the total birefringence $\Delta n$ for PS Runs No. 16 and 17 at mold temperature of 30 and 60 °C, at 4 cm from the sprue entrance. Measured $\Delta n$ near the outer wall did not show a significant increase when the mold temperature decreased. However, the thickness of the frozen-in $\Delta n$ increased when the mold temperature decreased, as evident in Fig. 8-42a at about $r/R=0.85$. Simulations showed a subtle increase of the total $\Delta n$ near the outer wall when the mold temperature decreased. This is due to the increase of the flow-induced birefringence near the outer wall when the mold temperature decreased. Near the inner wall, the simulated total $\Delta n$ increased when the mold temperature decreased. This was due to the higher thermally-induced birefringence generated during the faster cooling when the mold temperature decreased.
Figure 8-40 Measured (symbols) and simulated (lines) total $\Delta n$ for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 16 at mold temperature of 30 °C.
Figure 8-41 Measured (symbols) and simulated (lines) total $\Delta n$ for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 17 at mold temperature of 60 °C.
Figure 8-42 Measured (a) and simulated (b) total birefringence $\Delta n$ for Runs No. 16 and 17 at 4 cm from the sprue entrance, at mold temperatures of 30 and 60 ºC.

Figs. 8-43 and 8-44 show the measured and the simulated total birefringence, $n_{rr}$-$n_{\theta\theta}$, for PS Runs No. 16 and 17 at mold temperature of 30 and 60 ºC, respectively, at various distances from the sprue entrance: (a) and (b) in the sprue region at 4 and 6.5 cm, (c) and (d) in the primary gas penetration region of the spiral at 11 and 16 cm, and (e) in the solid region at 28 cm. For a mold temperature of 30 ºC, the maximum of the measured birefringence $n_{rr}$-$n_{\theta\theta}$ at the outer wall was higher than that of the measured $n_{rr}$-$n_{\theta\theta}$ at mold temperature of 60 ºC. The maximum of the simulated total birefringence, $n_{rr}$-$n_{\theta\theta}$, also decreased when the mold temperature increased. When the thermally-induced birefringence was added to the flow-induced birefringence, the total simulated $n_{rr}$-$n_{\theta\theta}$ for the mold temperature of 30 ºC showed a deeper minimum at about $r/R=0.85$ than that observed at the mold temperature of 60 ºC. This was due to the increase of the thermally-induced birefringence when the mold temperature decreased, due to the fast cooling.
Figure 8-43 Measured (symbols) and simulated (lines) total $n_{rr}-n_{\theta\theta}$ for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 16 at mold temperature of 30 °C.
Figure 8-44 Measured (symbols) and simulated (lines) total $n_{\theta\theta}-n_{rr}$ for a PS GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 6.5 cm, (c) at 11 cm, (d) at 16 cm, and (e) at 28 cm, for Run No. 17 at mold temperature of 60 ºC.
The high magnitude of the thermally-induced $n_{rr} - n_{\theta\theta}$ near the outer wall counterbalanced the flow-induced $n_{rr} - n_{\theta\theta}$. Therefore, the positive value of the thermally-induced $n_{rr} - n_{\theta\theta}$ dominated, creating the intermediate minimum.

8.3 Contribution of Thermal Birefringence in PC GAIM Moldings

This section presents the total simulated birefringence in PC GAIM moldings. The total birefringence comprises the thermally-induced birefringence, calculated according to the procedure explained in Section 4.5, and the flow-induced birefringence, previously shown in Chapter V.

Fig. 8-45 shows the measured birefringence $\Delta n$ and the simulated flow- and thermally-induced birefringence $\Delta n$, for PC Run No. 2 at various distances from the sprue entrance: (a) in the sprue region at 4 cm, (b) in the primary gas penetration region of the spiral at 16 cm, and (c) in the solid region at 48 cm. In the sprue region at 4 cm, the measured $\Delta n$ showed a maximum near the outer wall and decreased towards the inner wall showing plateau. In the primary gas penetration region of the spiral at the location of 16 cm, the measured $\Delta n$ showed a maximum near the outer wall, it decreased towards the inner wall passing through zero to a negative minimum. Then, the measured $\Delta n$ increased passing once more through zero to a positive maximum near the inner wall. In the solid region, at 48 cm, the measured $\Delta n$ showed a positive maximum near the outer wall, it decreased passing through zero to a negative minimum. Then $\Delta n$ increased passing again through zero to an extensive positive region in the core.
Figure 8-45 Measured (symbols) and simulated (lines) flow- and thermally-induced birefringence, $\Delta n$, for a PC tubular GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 48 cm, for Run No. 2, at a melt temperature of 280 ºC.

The simulated flow-induced $\Delta n$, at the location of 4 and 16 cm (Figs. 8-45a and b), showed a maximum near the outer wall. It decreased steeply toward the inner wall, where it relaxed almost completely. In the solid region (Fig. 8-45c), flow-induced $\Delta n$ showed a maximum near the outer wall. It decreased towards the center, where it relaxed almost completely. At 4 and 16 cm, the simulated thermally-induced $\Delta n$ showed a
negative minimum near the outer wall, it increased towards the inner wall passing through zero to positive value at the inner wall. In the solid region, the thermally-induced $\Delta n$ showed a negative minimum near the outer wall, it increased passing through zero to a positive value in the core. It is important to observe that, near the outer wall at the locations of 4 and 16 cm, the flow-induced $\Delta n$ was higher than the thermally-induced birefringence and they had opposite sign. When the thermally-induced birefringence $\Delta n$ was added to the flow-induced $\Delta n$, the total birefringence, shown in Fig. 8-46 at same distances from the sprue entrance as in Fig. 8-45, indicated that the contribution of the thermal birefringence for PC GAIM moldings was significant. At 4 cm, the simulated total birefringence $\Delta n$ showed a positive maximum near the outer wall, it decreased to a minimum and then increased towards the inner wall, showing a parabolic-like distribution. At 16 cm, the simulated total $\Delta n$ showed a maximum near the outer wall, it decreased passing through zero to a negative minimum, then, it increased towards the inner wall, passing once more through zero to a positive value at the inner wall. In the solid region, the total simulated $\Delta n$ also showed an intermediate maximum, it decreased toward the inner wall passing through zero to a negative minimum. After that, it increased passing once more through zero to an extensive positive value in the core region. For the PC GAIM moldings, it was found that the simulated flow-induced birefringence was significantly modified when the thermally-induced birefringence was included to calculate the total birefringence. This is because the magnitude of the simulated thermally-induced birefringence was significant.
Figure 8-46 Measured (symbols) and simulated (lines) total $\Delta n$, for a PC GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 48 cm, for Run No. 2.

Fig. 8-47 shows the measured birefringence $n_{rr}-n_{\theta\theta}$ and the simulated flow- and thermally-induced birefringence $n_{rr}-n_{\theta\theta}$ for PC Run No. 2 at various distances from the sprue entrance: (a) in the sprue region at 4 cm, (b) in the primary gas penetration region of the spiral at 16 cm, and (c) in the solid region at 48 cm.
Figure 8-47 Measured (symbols) and simulated (lines) flow- and thermally-induced birefringence, $n_{rr} - n_{\theta\theta}$, for a PC GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 48 cm, for Run No. 2.

At 4 cm from the sprue entrance, the absolute value of the simulated flow-induced $n_{rr} - n_{\theta\theta}$ was similar to that of the simulated thermally-induced birefringence. However, at 16 cm from the sprue entrance, the absolute value of the simulated flow-induced $n_{rr} - n_{\theta\theta}$ near the outer wall was smaller than the corresponding thermally-induced birefringence, $n_{rr} - n_{\theta\theta}$. They had opposite sign. For these two locations, near the inner wall, the flow-induced $n_{rr} - n_{\theta\theta}$ relaxed almost completely and the thermally-induced $n_{rr} - n_{\theta\theta}$ showed a
highest positive value. In the solid region, the simulated thermally-induced birefringence near the wall was significantly higher than the flow-induced birefringence. The low value of the flow-induced $n_{rr}-n_{θθ}$ was because the elasticity of the PC was lower than that of the PS. This can be observed in their respective viscosity curves (Figs. 5-1 and 5-2) where the PC showed a Newtonian behavior extensive to a higher shear rate than PS. This means that at low shear rate, the elasticity is not as important compared with that of the PS. Therefore, the first and second normal stress differences for PC were lower than those for PS.

When the thermally induced $n_{rr}-n_{θθ}$ was added to the flow-induced $n_{rr}-n_{θθ}$ the simulated total birefringence, shown in Fig. 8-48 at the same locations as in Fig. 8-47, showed large discrepancies. At 4 cm from the sprue entrance, (Fig. 8-48a) $n_{rr}-n_{θθ}$ showed an intermediate positive maximum near the outer wall, it decreased passing through zero to a negative minimum and increased passing once more through zero to a positive value at the inner wall. At the location of 16 cm, the simulated total birefringence showed a negative minimum near the outer wall while the measured $n_{rr}-n_{θθ}$ showed a positive maximum. In the solid region, the simulated total $n_{rr}-n_{θθ}$ showed a negative minimum near the outer wall, it increased passing through zero to a positive value in the core.

As evident in Fig 8-47, the large magnitude of the simulated thermally-induced birefringence on the PC GAIM moldings and the low contribution of the simulated flow-induced birefringence in the plane $r-θ$ led to large discrepancies between the total simulated and the measured $n_{rr}-n_{θθ}$. It might be possible that, due to the large contribution of thermally-induced birefringence for PC samples, adding the thermally-induced birefringence to the flow-induced birefringence considering free quenching was not
possible. Future calculations need to take into account the effect of constrained boundary conditions.

Figure 8-48 Measured (symbols) and simulated (lines) flow- and thermally-induced birefringence, \( n_{rr} - n_{\theta \theta} \), for a PC tubular GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 48 cm, for Run No. 2

8.4 Total Birefringence in PC GAIM Moldings

This section presents the influence of the injection speed at three different melt temperatures on the simulated total birefringence for PC GAIM moldings calculated according to the procedure shown in Section 4.5 and illustrated in Section 8.3.
Fig. 8-49, 8-50, and 8-51 show the measured and the simulated total birefringence, $\Delta n$, for PC Runs No. 1, 2, and 3 at injection speeds of 2.54 (1), 7.62 (3), and 15.24 (6) cm/s (in/s), respectively, for a melt temperature of 280 °C, at various distances from the sprue entrance: (a) in the sprue region at 4 cm, (b) in the primary gas penetration region of the spiral at 16 cm, and (c) in the solid region at 48 cm. The simulated total birefringence $\Delta n$ increased with injection speed. Furthermore, the frozen-in layer decreased when the injection speed increased. Near the outer wall, the magnitude of the thermally-induced birefringence was higher for PC GAIM moldings than for the PS GAIM moldings. Therefore, when the contribution of the simulated thermally-induced birefringence was added to the simulated flow-induced birefringence, the total birefringence showed a very low magnitude near the outer wall. At 16 cm from the sprue entrance, the simulated total birefringence $\Delta n$ showed a maximum close to the outer wall. It decreased towards the inner wall showing a minimum. Then, the birefringence increased towards the inner wall. In the solid region, the total simulated birefringence showed a maximum close to the outer wall and decreased towards the core showing an extensive region of positive birefringence. When the injection speed increased, the contribution of the flow-induced birefringence increased. However, the magnitude of the thermally-induced birefringence remained in the same range, since the thermally-induced birefringence was mainly generated when the polymer passed through $T_g$ during cooling. Therefore, for a high injection speed, the flow-induced birefringence increased due to the increase of the shear and normal stresses difference. Therefore, the intermediate maximum near the outer wall and the minimum of the simulated total $\Delta n$ shifted towards the outer wall.
Figure 8-49 Measured (symbols) and simulated (lines) total birefringence, $\Delta n$, for a PC GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 60 cm, for Run No. 1, at injection speed of 2.54 cm/s.
Figure 8-50 Measured (symbols) and simulated (lines) total birefringence, \( \Delta n \), for a PC GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 48 cm, for Run No. 2, at injection speed of 7.62 cm/s.
Figure 8-51 Measured (symbols) and simulated (lines) total birefringence, $\Delta n$, for a PC GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 48 cm, for Run No. 3 at injection speed of 15.24 cm/s.

Figs. 8-52, 8-53, and 8-54 show the measured and simulated total birefringence, $n_{rr} - n_{00}$, for PC Runs No. 1, 2, and 3 at injection speeds of 2.54 (1), 7.62 (3), and 15.24 (6) cm/s (in/s), respectively, at various distances from the sprue entrance: (a) in the sprue region at 4 cm, (b) in the primary gas penetration region of the spiral at 16 cm, and (c) in the solid region at 48 cm. The simulated total $n_{rr} - n_{00}$ showed an intermediate maximum near the outer wall, decreased to a minimum, and then increased towards the inner wall to
the highest positive value. It is important to note that the minimum of the total simulated birefringence at 4 cm from the sprue entrance decreased when the injection speed increased. This is because, when the injection speed increased, the thickness of the frozen-in layer of the flow induced \( n_{rr} - n_{\theta\theta} \) decreased. Therefore, the contribution of the thermally-induced birefringence further away from the frozen-in layer of \( n_{rr} - n_{\theta\theta} \) became dominant, rendering a negative minimum.

Figure 8-52 Measured (symbols) and simulated (lines) total birefringence, \( n_{rr} - n_{\theta\theta} \), for a PC tubular GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 48 cm, for Run No. 1.
Figure 8-53 Measured (symbols) and simulated (lines) total birefringence, $n_{rr} - n_{\theta\theta}$, for a PC GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 48 cm, for Run No. 2.
Figure 8-54 measured (symbols) and simulated (lines) total birefringence, $n_{rr} - n_{00}$, for a PC GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 48 cm, for Run No. 3.

Figs. 8-55, 8-56, and 8-57 show the measured and simulated total birefringence, $\Delta n$, for PC Runs No. 4, 5, and 6, at injection speeds of 2.54 (1), 7.62 (3), and 15.24 (6) cm/s (in/s), respectively, for a melt temperature of 300 °C, at various distances from the sprue entrance: (a) in the sprue region at 4 cm, (b) in the primary gas penetration region of the spiral at 16 cm, and (c) in the solid region at 48 cm. In general, by increasing the
melt temperature from 280 to 300 °C, the simulated total birefringence decreased for a specific injection speed. This is because the flow-induced birefringence decreased when the melt temperature increased, as discussed in Section 6.4.1. The simulated total birefringence $\Delta n$ increased with injection speed. This is because the shear and normal stresses increased during the filling stage, as discussed in Section 6.4.4.

![Graphs showing measured and simulated total birefringence](image)

Figure 8-55 Measured (symbols) and simulated (lines) total birefringence, $\Delta n$, for a PC GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 60 cm, for Run No. 4, at injection speed of 2.54 cm/s.
Figure 8-56 Measured (symbols) and simulated (lines) total birefringence, $\Delta n$, for a PC tubular GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 60 cm, for Run No. 5, at injection speed of 7.62 cm/s.
Figure 8-57 Measured (symbols) and simulated (lines) total birefringence, $\Delta n$, for a PC tubular GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 60 cm, for Run No. 6, at injection speed of 15.24 cm/s.

Simulated total $\Delta n$ showed that the thickness of the frozen-in $\Delta n$ decreased when the injection speed increased. In the solid region, the simulated total birefringence showed a negative minimum. This minimum became lower when the injection speed increased. This is because at high injection speed, the thickness of the frozen-in layer of the flow-induced birefringence decreased and the negative portion of the thermally-
induced birefringence near the outer wall became dominant. The maximum of the
simulated total $\Delta n$ near the outer wall increased with the injection speed. This is because,
when the injection speed increased, the simulated flow-induced $\Delta n$ increased. Meanwhile
the magnitude of the thermally-induced birefringence remained in the same range. When
the thermally- and flow-induced birefringence components were added, they rendered a
higher maximum intermediate of $\Delta n$.

Figs. 8-58, 8-59, and 8-60 show the measured and the simulated total
birefringence, $n_{rr}-n_{\theta\theta}$, for PC Runs No. 4, 5, and 6 at injection speeds of 2.54 (1), 7.62 (3),
and 15.24 (6) cm/s (in/s) at a melt temperature of 300 °C, respectively, at various
distances from the sprue entrance: (a) in the sprue region at 4 cm, (b) in the primary gas
penetration region of the spiral at 16 cm, and (c) in the solid region at 48 cm. In general,
by increasing the melt temperature, the flow-induced birefringence decreased but the
thermally-induced birefringence increased. As a consequence, the total simulated $n_{rr}-n_{\theta\theta}$
at lower melt temperature showed a lower magnitude near the outer wall when compared
at the same injection speed. Nevertheless, by increasing the injection speed, the flow-
induced birefringence near the outer wall increased. Accordingly, the simulated total $\Delta n$
increased with injection speed.

Fig. 8-61, 8-62, and 8-63 show the measured and the simulated total
birefringence, $\Delta n$, for PC Runs No. 7, 8, and 9 at injection speeds of 2.54 (1), 7.62 (3),
and 15.24 (6) cm/s (in/s), respectively, for a melt temperature of 320 °C, at various
distances from the sprue entrance: (a) in the sprue region at 4 cm, (b) in the primary gas
penetration region of the spiral at 16 cm, and (c) in the solid region at 48 cm.
Figure 8-58 Measured (symbols) and simulated (lines) total birefringence, $n_{rr} - n_{00}$, for a PC GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 48 cm, for Run No. 4 at injection speed of 2.54 cm/s and melt temperature of 300 °C.
Figure 8-59 Measured (symbols) and simulated (lines) total birefringence, $n_{rr} - n_{\theta\theta}$, for a PC GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 48 cm, for Run No. 5 at injection speed of 7.64 cm/s and a melt temperature of 300 ºC.
Figure 8-60 Measured (symbols) and simulated (lines) total birefringence, \( n_{rr} - n_{\theta\theta} \), for a PC GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 48 cm, for Run No. 6 at injection speed of 15.24 cm/s and melt temperature of 300 °C.
Figure 8-61 measured (symbols) and simulated (lines) total birefringence, $\Delta n$, for a PC GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 60 cm, for Run No. 7, at injection speed of 2.54 cm/s and melt temperature of 320 °C
Figure 8-62 Measured (symbols) and simulated (lines) total birefringence, $\Delta n$, for a PC GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 60 cm, for Run No. 8, at injection speed of 7.62 cm/s and melt temperature of 320 ºC.
Figure 8-63 Measured (symbols) and simulated (lines) total birefringence, $\Delta n$, for a PC GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 60 cm, for Run No. 9, at injection speed of 15.24 cm/s and melt temperature of 320 °C.
The total simulated birefringence $\Delta n$ increased with the injection speed. Furthermore, for a specific injection speed, the simulated total $\Delta n$ decreased when the melt temperature increased, as discussed in Section 6.4.1. The thermally-induced birefringence also increased with the melt temperature and became dominant near the outer wall. This rendered a negative minimum of the simulated total $\Delta n$ near the outer wall, that decreased when the injection speed increased.

Fig. 8-64, 8-65, and 8-66 show the measured and the simulated total birefringence, $n_{rr} - n_{\theta\theta}$, for PC Runs No. 7, 8, and 9 at injection speeds of 2.54 (1), 7.62 (3), and 15.24 (6) cm/s (in/s), respectively, for a melt temperature of 320 ºC at various distances from the sprue entrance: (a) in the sprue region at 4 cm, (b) in the primary gas penetration region of the spiral at 16 cm, and (c) in the solid region at 48 cm. In general, for the same injection speed, the simulated total birefringence, $n_{rr} - n_{\theta\theta}$, decreased when the melt temperature increased. As explained before, the flow-induced birefringence decreased when the melt temperature increased. The contribution of the thermally-induced negative birefringence, which increased with the melt temperature, became dominant. Accordingly, when both flow- and thermally induced $n_{rr} - n_{\theta\theta}$ were added, the total simulated birefringence $n_{rr} - n_{\theta\theta}$ showed a negative minimum near the outer wall for the three injection speeds employed.
Figure 8-64 Measured (symbols) and simulated (lines) total birefringence, $n_{rr} - n_{\theta\theta}$, for a PC GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 48 cm, for Run No. 7 at injection speed of 2.54 cm/s and melt temperature of 320 ºC.
Figure 8-65 measured (symbols) and simulated (lines) total birefringence, $n_{rr} - n_{00}$, for a PC GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 48 cm, for Run No. 8 at injection speed of 7.62 cm/s and melt temperature of 320 °C.
Figure 8-66 Measured (symbols) and simulated (lines) total birefringence, $n_{rr} - n_{\theta\theta}$, for a PC GAIM molding at various distances from the sprue entrance: (a) at 4 cm, (b) at 16 cm, and (c) at 48 cm, for Run No. 9 for an injection speed of 15.24 cm/s and melt temperature of 320 °C.

8.5 Total Average Birefringence in PS GAIM Moldings Contribution of Thermally-Induced Birefringence.

This section contrasts the total simulated and measured average birefringence $<n_{zz} - n_{\theta\theta}>$ in PS GAIM moldings. The simulated thermally-induced birefringence was
added to the simulated flow-induced birefringence to obtain the total simulated average birefringence. Figs. 8-67, 8-68, 8-69, 8-70, 8-71, and 8-72 show the measured and simulated total birefringence for PS GAIM moldings at various melt temperatures, shot sizes, injection speeds, gas-delay time, and mold temperatures. Simulations showed that the contribution of thermally-induced birefringence in PS GAIM moldings was much lower than the flow-induced average birefringence. Therefore, for the PS GAIM moldings the flow-induced birefringence was the main factor causing residual birefringence. Comparing Figs. 5-111 to 5-114 with Figs. 8-67 to 8-72, it is observed that the total simulated birefringence was not significantly different from the flow-induced average birefringence, since the contribution of the thermal birefringence was not significant for PS as discussed in Chapter VI.

Figure 8-67 Measured (symbols) and simulated (lines) total average birefringence \(<n_{zz} - n_{\theta\theta}>\) with respect to the distance from the sprue entrance for PS Runs No. 1, 2, and 3.
Figure 8-68 Measured (symbols) and simulated (lines) total average birefringence $<n_{zz} - n_{θθ}>$ with respect to the distance from the sprue entrance for PS Runs No. 4, 5, and 6.

Figure 8-69 Measured (symbols) and simulated (lines) total average birefringence $<n_{zz} - n_{θθ}>$ with respect to the distance from the sprue entrance for PS Runs No. 7, 8, and 9.
Figure 8-70 Measured (symbols) and simulated (lines) total average birefringence $<n_{zz} - n_{θθ}>$ with respect to the distance from the sprue entrance for PS Runs No. 10, 11, and 12.

Figure 8-71 Measured (symbols) and simulated (lines) total average birefringence $<n_{zz} - n_{θθ}>$ with respect to the distance from the sprue entrance for PS Runs No. 13, 14, and 15.
Figure 8-72 measures (symbols) and simulated (lines) total average birefringence \( <n_{zz} - n_{θθ}> \) with respect to the distance from the sprue entrance for PS Runs No. 16 and 17.

8.6 Total Average Birefringence in PC GAIM Moldings Contribution of Thermally-Induced Birefringence.

Fig. 5-73 shows the measured and simulated total average birefringence in PC GAIM moldings for PC Runs No. 1, 2, and 3 made at various injection speeds. The simulated total birefringence \( <n_{zz} - n_{θθ}> \) showed that the contribution of the thermally-induced birefringence was significant. This was especially evident in the solid region, where the thermally-induced birefringence was dominant over the flow-induced birefringence. The simulated flow-induced average birefringence was very low (as shown in Fig. 5-117). This was because the thickness of the frozen birefringence layer was lower. Therefore, when the birefringence was averaged over the RWT, the magnitude of the flow-induced birefringence became low. However, simulations and free quenching experiments (shown in Chapter VI) demonstrated that the magnitude of the thermally-
induced birefringence in PC samples was significant. Therefore, it is observed in Fig. 8-73 that the birefringence in the solid region was higher than the birefringence in the primary gas penetration region of the spiral. This behavior is totally opposite to that observed in PS GAIM moldings, where the total birefringence of the solid region was lower than the total average birefringence of the primary gas penetration region.

![Figure 8-73](image)

Figure 8-73 Measure (symbols) and simulated (lines) total average birefringence $<n_{zz} - n_{θθ}>$ with respect to the distance from the sprue entrance for PC Runs No. 1, 2, and 3.

8.7 Conclusions

Simulations of the flow- and thermally-induced birefringence $\Delta n$ and $n_{zz} - n_{θθ}$, for PS GAIM moldings showed that the birefringence near the outer wall was mainly caused by flow during the filling stage. Simulations of the thermally-induced birefringence showed that the birefringence near the inner wall and in the core region of the PS GAIM moldings was mainly caused by thermal stresses generated during cooling. Simulations demonstrated that the thermal birefringence, $\Delta n$, in GAIM moldings was one order of
magnitude lower than the flow-induced birefringence. However, the flow- and thermally-
induced birefringence, $n_{rr} - n_{\theta\theta}$, had the same order of magnitude. Then, combining the
flow- and thermally-induced birefringence calculated for GAIM molding of PS, showed a
better description of the measured birefringence. This observation was supported by the
annealing experiments in PS GAIM moldings shown in Section 6.9. The birefringence
near the inner wall relaxed during the annealing process while the birefringence near the
outer wall did not relax in the same proportion. For the case of PC moldings, the
contribution of the thermally-induced birefringence was significant throughout the RWT.
In the sprue region, the flow-induced birefringence was higher than the thermally-
induced birefringence. However, in the spiral region, the magnitude of the flow- and
thermally-induced birefringence near the outer wall was almost of the same order of
magnitude. This caused a large deviation between the total simulated birefringence and
the measured birefringence.
CHAPTER IX
SUMMARY

Measurements and viscoelastic simulations of polymer/gas interface distribution, the radial distribution of the birefringence components, \( \Delta n \) and \( n_{rr}-n_{\theta\theta} \), and the average birefringence, \( \langle n_{zz}-n_{\theta\theta} \rangle \) were carried out on PS and PC GAIM moldings obtained under various processing conditions. Furthermore, measurements and viscoelastic simulations of the birefringence components were carried out in freely quenched tubes and rods of PS and PC. The importance of numerical simulations in both mold and process design, make the viscoelastic numerical scheme developed in the present dissertation an important tool to calculate the influence of the processing variables on the distribution of the polymer/gas interface and the contributions of the flow- and thermally-induced birefringence components in GAIM moldings. To model the polymer/gas interface distribution, the gas was replaced by a fictitious fluid and the conservation equations for both the polymer and gas domains were solved using a hybrid numerical scheme based on finite elements/control volume/finite difference. Flow- and thermally-induced stresses were calculated using, respectively, nonlinear and linear viscoelastic theories. The flow-induced birefringence was calculated from the flow-induced stresses using the stress-optical rule. The thermally-induced birefringence was calculated using a photoviscoelastic theory. The numerical scheme simulated the pressure traces during the
GAIM process. However, the simulated cavity pressure was higher than the measured cavity pressure. This difference was attributed to the formation of the frozen layer of polymer during the filling stage. This was evident from the cavity pressure measured during the gas penetration stage, which was significantly lower than the gas pressure. The present formulation was able to predict in a qualitative manner the effect of processing variables on the polymer/gas interface distribution. According to the simulated results, it can be concluded that the RWT and gas penetration length was influenced directly by the melt temperature profile that existed prior to the gas penetration. This is because all the processing variables influenced directly the temperature distribution of the melt which determines the viscosity distribution prior to the gas injection. Even though the viscosity of the polymer has a complex interrelation with temperature and shear rate, it was found that those processing variables that rendered a lower temperature distribution prior to gas penetration caused the RWT to increase. Accordingly low mold temperature, low injection speed, low melt temperature, and long gas-delay time increased the RWT. On the other hand, the processing variables that affected the melt rheology such as gas pressure also modified the RWT. The most influential processing variables that affected the RWT in the PS GAIM moldings were the gas-delay time and the injection speed. In both cases, the temperature distribution along the radius of the molding played an important role. Long delay time caused a larger drop in the temperature, as a consequence, the solid layer of polymer formed near the mold wall before the gas injection increased, reducing the area available for the gas to penetrate. In the instance when low injection speed was used, the high filling time and the low viscous dissipation led also to a drop of the melt temperature prior to gas injection. Therefore, the area
available for the gas penetration reduced also. The most influential variable in the gas penetration length was the shot size. This was evident since the volume available for the gas to penetrate increased when the shot size decreased. However, it did not exert a definite influence on the RWT except for the large shot size. The injection speed and the gas-delay time also exerted a strong influence on the gas penetration length. This was because low injection speed and long gas-delay time increased the RWT. Therefore, owing to constant volume of the cavity, the gas penetration length increased.

Among the processing conditions studied for PS moldings, it was found that the injection speed was one of the variables that exerted strong influence on RWT, gas penetration length, and birefringence. Low injection speed renders thicker RWT, longer gas penetration length, and thicker frozen-in birefringence layer.

For PC GAIM moldings obtained at the three melt temperatures, measurements and simulations showed that the RWT and gas penetration length decreased when injection speed increased. However, discrepancies were observed between measurements and simulations. Furthermore, simulated polymer/gas interface distribution showed oscillations. These oscillations were reduced when the number of meshes along the radius was increased. However, due to the increase of computation time, further decrease in mesh size was not possible.

The numerical scheme described the development of birefringence, $\Delta n$, during the filling and gas penetration stages of GAIM and simulated the residual birefringence distribution $\Delta n$ and $n_{rr}-n_{\theta\theta}$ along the radial direction, and the average birefringence $<n_{zz}-n_{\theta\theta}>$ along the flow direction of GAIM moldings. Simulations qualitatively described the effect of processing variables on residual birefringence components in GAIM moldings.
The measured birefringence, $\Delta n$ and $n_{rr}-n_{\theta\theta}$, for PS GAIM moldings showed a maximum near the outer wall. Then they decreased towards the inner wall showing a plateau. This maximum of $\Delta n$ observed near the outer wall varied among the different regions along the tubular moldings. The maximum of $\Delta n$ in the sprue region was higher than that in the primary gas penetration region of the spiral. In the solid region the maximum of $\Delta n$ showed its lowest value. Simulations showed that the low magnitude of $\Delta n$ in the spiral region was due to its bigger diameter compared to that of the sprue. The bigger diameter of the spiral led to lower shear and normal stresses, as a consequence, to lower birefringence.

For PS GAIM moldings, simulations indicated that the birefringence at the outer wall was mainly caused by the frozen-in molecular orientation during the filling stage and it was highly influenced by the processing conditions while the birefringence near the inner wall was caused by the thermal stresses generated during the cooling stage. Simulations also indicated that during the gas penetration stage, the birefringence profile generated during the filling stage partially relaxed but it was, to lesser degree influenced by the processing conditions prevailing during the gas penetration, since the gas pressure was significantly lower than the injection pressure.

The processing variables that exerted most influence on the measured birefringence $\Delta n$ in PS GAIM moldings were the melt temperature, the gas-delay time and the injection speed. The mold temperature, the shot size, and gas pressure exerted little influence on the flow-induced residual birefringence at least within the processing window employed. Simulations agreed qualitatively with measurements. It was found that the birefringence decreased when the melt temperature increased. This was due to the
reduction of the viscosity and the decrease of relaxation time of the polymer. The second most important factor was the injection velocity, high injection velocity leads to higher birefringence near the wall but at the same time leads to a thinner frozen-in birefringence layer. At low injection speed the maximum of the birefringence decreased but the thickness of the frozen-in birefringence increased due to cooling.

Simulations and experiments carried out in PS GAIM moldings showed that by increasing the gas-delay time, a second intermediate maximum appeared due to the stresses generated during the gas penetration stage. This increased the overall residual birefringence. However, because of the increase in the RWT, the average birefringence \( <n_{zz}n_{\theta\theta}> \) decreases in comparison with that observed in molded samples with no gas-delay time.

Experiments and simulations showed that a decrease of the mold temperature caused an increase in the frozen-in birefringence. This was due to the increase of the heat removal rate when the mold temperature decreased. It was found that the shot size exerted little influence on the measured birefringence within the processing window used in this study.

The measured \( n_{rr}-n_{\theta\theta} \) for PS GAIM moldings was found to be one order of magnitude lower than \( \Delta n \) for all the processing conditions and all the locations of the spiral analyzed. However, for PC GAIM moldings, the magnitude of the birefringence \( n_{rr}-n_{\theta\theta} \) was of the same order of magnitude of \( \Delta n \) in the primary gas penetration region of the spiral. Simulations of the flow-induced birefringence showed that the magnitude of the birefringence \( n_{rr}-n_{\theta\theta} \) was always lower than the magnitude of flow-induced \( \Delta n \). The thermally-induced residual birefringence for PS GAIM moldings was one order of magnitude lower.
magnitude lower than the flow-induced birefringence. However, for the PC GAIM moldings the thermally-induced birefringence was of the same order as the flow-induced residual birefringence. This is why the magnitude of \( \Delta n \) and \( n_{rr} - n_{\theta\theta} \) were comparable in the case of PC GAIM moldings.

The influence of the processing parameters on the average birefringence \( \langle n_{zz} - n_{\theta\theta} \rangle \) along the length of the GAIM moldings was studied. It was found that the most important parameters affecting the average birefringence were the melt temperature and the gas-delay time, followed by the injection speed. The mold temperature, shot size, and gas pressure were the processing parameters that exerted less influence on the average birefringence. However, it was observed that the average birefringence showed a larger plateau when the shot size decreased, due to the increase of the gas penetration length.

Measured average birefringence for PS GAIM moldings indicated that it decreased in the sprue, showed a plateau in the primary gas penetration region of the spiral and decreased in the solid section. Simulations also indicated that for the PS GAIM moldings, the main contribution to the average birefringence was caused by the flow-induced birefringence. Simulations qualitatively described the behavior of the average birefringence along the GAIM moldings. However, the minimum observed in the average birefringence between the primary and secondary gas penetration regions was not described by the present approach. This minimum was attributed to the stress relaxation in the proximity of the solid region of the spiral, possibly due to the high temperature in this region.

It was found that the sample annealing at temperature below the glass transition temperature caused the birefringence near the inner wall to relax and that near the outer wall to remain unrelaxed. The hypothesis that the birefringence at the inner wall was
created by thermally-induced residual stresses is supported by the fact that the birefringence relaxed below the $T_g$. The free volume in glassy polymers increases during fast quenching. Accordingly, it was clear that increase of free volume in glassy polymers permits better segmental mobility, leading to earlier softening, and as a consequence, the stresses relaxation.

Because of the little change of the birefringence near the outer wall after annealing the sample, it can be concluded that the main cause of birefringence near the wall is the flow-induced stresses during the filling stage and cooling.

When a section of the PC GAIM molding was annealed below $T_g$, the birefringence in both near the inner and outer walls decreased. This indicated that the thermal stresses exert a strong influence throughout the wall thickness of the PC GAIM moldings.

Simulations indicated that flow birefringence induced during the gas penetration stage was lower than that induced during the filling stage. This is because the high injection pressure leads to high shear and normal stresses during the filling stage and the low mold temperature cools the polymer near the mold wall leading to the frozen-in birefringence of a high magnitude. Conversely, the birefringence relaxes in the core region due to the high temperature of the polymer melt in the core leading to a fast relaxation of flow-induced stresses.

The thickness of the slices cut from the PC GAIM moldings to measure the birefringence exerted a strong influence on the distribution of $\Delta n$ and $n_{rr-n_{\theta\theta}}$. For the case of PS, the birefringence $\Delta n$ did not change significantly between slice thickness of 0.5 and 1 mm. However the birefringence $n_{rr-n_{\theta\theta}}$ did show a higher variation than that
observed for \( \Delta n \). Nevertheless, the magnitude was in the same range. However, for the PC GAIM moldings the birefringence \( \Delta n \) and \( n_{rr} - n_{\theta\theta} \) was significantly altered when the slice thickness was varied.

At low initial quenching temperature, simulated birefringence for PS tubes and rods showed a large deviation from measurements. This could be attributed to thermally-induced stresses in the elastic range, since at an initial temperature close to \( T_g \), the molecules could have been quickly frozen and the long-range molecular motion was hindered. This could have led to a segmental orientation and bond deformation, in turn causing changes in birefringence when the slice was removed from the sample. However, the question remains open and further investigation will be needed in order to understand this effect. When the initial quenching temperature of the PS samples was increased, the simulated birefringence showed a better agreement with experiments. This can be attributed to the increase of molecular mobility at a high temperature. This could have led to an increase of the long-range molecular orientation that remained after the slice was removed from the quenched sample.

In general, the magnitude of thermally-induced birefringence of free-quenched tubes and rods of PC was higher than that for PS samples. This was because the strain-optical coefficient of PC was higher than that of the PS near the glass transition temperature. However, the magnitude of the simulated residual stresses for tubes and rods of PS was higher than that for the corresponding PC samples. This was because the stress relaxation of the PC was more significant than the stress relaxation of PS.

By adding the flow- and thermally-induced birefringence for PS GAIM moldings, simulations showed a better description of the measured birefringence. However, for the
case of PC moldings, simulations showed large discrepancies. This was attributed to the strong contribution of the thermally-induced birefringence throughout the RWT.
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APPENDIX A

DISCRETIZATION OF THE LINEAR MODEL TO CALCULATE THE THERMALLY-INDUCED STRESSES

This appendix shows the procedure utilized to discretize the equations of the stress components (Eq-4-14) of the linear model used to calculate the thermally-induced stresses.

The radial component of the thermal stresses, $\sigma_{rr}$, is written as:

$$
\sigma_{rr}(r, \xi_n(r)) = \int_0^\infty \frac{2}{3} G(\xi_n - \xi_n) \frac{d}{d\xi_n} \left[ 2\varepsilon_n(\xi_n) - \varepsilon_n(\xi_n) - \varepsilon_{\infty}(\xi_n) \right] d\xi_n 
+ \int_0^\infty K(\xi_n - \xi_n) \frac{d}{d\xi_n} \left[ \varepsilon_n(\xi_n) + \varepsilon_n(\xi_n) + \varepsilon_{\infty}(\xi_n) - 3\varepsilon_{\infty}(\xi_n) \right] d\xi_n
$$

(A-1)

Expanding Eq. A-1 and using integration by parts of the form:

$$
\frac{d}{d\xi_n}(\varepsilon_n) \quad \text{and} \quad dG(\xi_n - \xi_n)
$$

(A-2)

Neglecting the terms that contain second order derivatives that result from the integration by parts, we can approximate equation (A-1) as:

$$
\sigma_{rr}(r, \xi_n(r)) = \frac{2}{3} \frac{d}{d\xi_n} \left[ 2\varepsilon_n(\xi_n) - \varepsilon_n(\xi_n) - \varepsilon_{\infty}(\xi_n) \right] \int_0^\infty G(\xi_n - \xi_n) d\xi_n 
+ \frac{d}{d\xi_n} \left[ \varepsilon_n(\xi_n) + \varepsilon_n(\xi_n) + \varepsilon_{\infty}(\xi_n) - 3\varepsilon_{\infty}(\xi_n) \right] \int_0^\infty K(\xi_n - \xi_n) d\xi_n
$$

(A-3)
The integrals are discretized using the trapezoidal rule yielding a step function which is constant over each interval (piecewise linear approximation), the derivatives with respect to the reduced time are discretized using backward difference yielding:

\[
\sigma_n^{i,j}(r, \xi_n(t)) = \sum_{\nu=1}^{3} \left[ 2 \varepsilon_n^{\nu,j} - 2 \varepsilon_n^{\nu,j-1} \right] - (\varepsilon_n^{\nu,j} - \varepsilon_n^{\nu,j-1}) - (\varepsilon_n^{\nu,j} - \varepsilon_n^{\nu,j-1}) \right] \cdot \frac{1}{\xi_n} \int_{\xi_n}^{\xi_n} G(\xi - \xi_n) \xi d\xi \\
+ \sum_{\nu=1}^{3} \left[ (\varepsilon_n^{\nu,j} - \varepsilon_n^{\nu,j-1}) + (\varepsilon_n^{\nu,j} - \varepsilon_n^{\nu,j+1}) + (\varepsilon_n^{\nu,j} - \varepsilon_n^{\nu,j+1}) - 3(\varepsilon_n^{\nu,j} - 3\varepsilon_n^{\nu,j+1}) \right] \cdot \frac{1}{\xi_n} \int_{\xi_n}^{\xi_n} K(\xi - \xi_n) \xi d\xi 
\]

(A-4)

For the sake of simplicity the following definition is employed:

\[
\Gamma_n^{i,j} = \frac{1}{\xi_n} \int_{\xi_n}^{\xi_n} G(\xi - \xi_n) \xi d\xi \\
K_n^{i,j} = \frac{1}{\xi_n} \int_{\xi_n}^{\xi_n} K(\xi - \xi_n) \xi d\xi
\]

(A-5)

Evaluating the summation at present time \( k=j \) and grouping the strain, \( \varepsilon \), terms for the present time, equation (A-4) can be rewritten as:

\[
\sigma_n^{i,j} = \varepsilon_n^{i,j} \left[ \frac{4}{3} \Gamma_n^{i,j} + K_n^{i,j} \right] + \varepsilon_n^{i,j} \left[ K_n^{i,j} - \frac{2}{3} \Gamma_n^{i,j} \right] + \varepsilon_n^{i,j} \left[ K_n^{i,j} - \frac{2}{3} \Gamma_n^{i,j} \right] \\
+ \frac{2}{3} \Gamma_n^{i,j} \left[ -2 \varepsilon_n^{i,j} + \varepsilon_n^{i,j+1} + \varepsilon_n^{i,j+1} \right] + \sum_{\rho=1}^{3} \frac{2}{3} \Gamma_n^{i,j} \left[ 2 \varepsilon_n^{i,j} - 2 \varepsilon_n^{i,j} + \varepsilon_n^{i,j+1} \right] \\
+ K_n^{i,j} \left[ 3 \varepsilon_n^{i,j} - 3 \varepsilon_n^{i,j} - \varepsilon_n^{i,j+1} \right] \\
+ \sum_{\rho=1}^{3} K_n^{i,j} \left[ \varepsilon_n^{i,j} - \varepsilon_n^{i,j+1} + \varepsilon_n^{i,j} - \varepsilon_n^{i,j+1} - 3 \varepsilon_n^{i,j} + 3 \varepsilon_n^{i,j+1} \right] 
\]

(A-6)

for the sake of simplicity the following variables are defined:
\[ C_i = \left[ \frac{4}{3} \Gamma^{i,j} + K^{i,j} \right] \]

\[ C_2 = \left[ K^{i,j} - \frac{2}{3} \Gamma^{i,j} \right] \]

\[ C_3 = \frac{2}{3} \Gamma^{i,j} \left[ -2 \varepsilon^{i,j}_{nr} + \varepsilon^{i,j}_{nn} + \varepsilon^{i,j}_{zz} \right] + \sum_{k=1}^{N} \frac{2}{3} \Gamma^{k,i} \left[ 2 \varepsilon^{i,k}_{rr} - 2 \varepsilon^{i,k}_{nn} + \varepsilon^{i,k}_{zz} \right] \]

\[ + \sum_{k=1}^{N} K^{k,i} \left[ 3 \varepsilon^{i,k}_{rr} - 3 \varepsilon^{i,k}_{nn} + \varepsilon^{i,k}_{zz} \right] \]

\[ + \sum_{j=1}^{N} K^{i,j} \left[ \varepsilon^{i,j}_{rr} - \varepsilon^{i,j}_{nn} + \varepsilon^{i,j}_{zz} \right] \]

Then, Eq. (A-6) reduces to:

\[ \sigma_{rr}^{ij} = C_i \varepsilon_{rr}^{ij} + C_2 \left( \varepsilon_{nn}^{ij} + \varepsilon_{zz}^{ij} \right) + C_3 \]

Following the same procedure for the stresses in circumferential, \( \sigma_{\theta \theta} \), and axial direction, \( \sigma_{zz} \), we obtain:

\[ \sigma_{\theta \theta}^{ij} = C_4 \varepsilon_{\theta \theta}^{ij} + C_2 \left( \varepsilon_{rr}^{ij} + \varepsilon_{zz}^{ij} \right) + C_4 \]

\[ \sigma_{zz}^{ij} = C_5 \varepsilon_{zz}^{ij} + C_2 \left( \varepsilon_{rr}^{ij} + \varepsilon_{\theta \theta}^{ij} \right) + C_5 \]

where the variables \( C_4 \) and \( C_5 \) are defined as:

\[ C_4 = \frac{2}{3} \Gamma^{i,j} \left[ -2 \varepsilon^{i,j}_{\theta \theta} + \varepsilon^{i,j}_{rr} + \varepsilon^{i,j}_{zz} \right] + \sum_{k=1}^{N} \frac{2}{3} \Gamma^{k,i} \left[ 2 \varepsilon^{i,k}_{rr} - 2 \varepsilon^{i,k}_{\theta \theta} + \varepsilon^{i,k}_{zz} \right] \]

\[ + \sum_{k=1}^{N} K^{k,i} \left[ 3 \varepsilon^{i,k}_{rr} - 3 \varepsilon^{i,k}_{\theta \theta} + \varepsilon^{i,k}_{zz} \right] \]

\[ + \sum_{j=1}^{N} K^{i,j} \left[ \varepsilon^{i,j}_{rr} - \varepsilon^{i,j}_{\theta \theta} + \varepsilon^{i,j}_{zz} \right] \]

\[ C_5 = \frac{2}{3} \Gamma^{i,j} \left[ -2 \varepsilon^{i,j}_{zz} + \varepsilon^{i,j}_{rr} + \varepsilon^{i,j}_{\theta \theta} \right] + \sum_{k=1}^{N} \frac{2}{3} \Gamma^{k,i} \left[ 2 \varepsilon^{i,k}_{zz} - 2 \varepsilon^{i,k}_{\theta \theta} + \varepsilon^{i,k}_{rr} \right] \]

\[ + \sum_{k=1}^{N} K^{k,i} \left[ 3 \varepsilon^{i,k}_{zz} - 3 \varepsilon^{i,k}_{\theta \theta} + \varepsilon^{i,k}_{rr} \right] \]

\[ + \sum_{j=1}^{N} K^{i,j} \left[ \varepsilon^{i,j}_{rr} - \varepsilon^{i,j}_{\theta \theta} + \varepsilon^{i,j}_{zz} \right] \]

\[ C_5, C_4 \text{ and } C_5 \text{ keep the stress history and they are function of the radius as well.} \]
APPENDIX B

TIME STEP FOR THERMALLY-INDUCED RESIDUAL STRESS CALCULATIONS

0.000, 0.0001, 0.0002, 0.0004, 0.0006, 0.0008, 0.0010, 0.0012, 0.0014, 0.0016
0.0018, 0.0020, 0.0025, 0.0030, 0.0035, 0.0040, 0.0045, 0.0050, 0.0055, 0.0060
0.0065, 0.0070, 0.0075, 0.0080, 0.0085, 0.0090, 0.0095, 0.0100, 0.0110, 0.0120
0.013, 0.014, 0.015, 0.016, 0.017, 0.018, 0.019, 0.020, 0.021, 0.022, 0.023, 0.024
0.025, 0.026, 0.027, 0.028, 0.029, 0.030, 0.032, 0.034, 0.036, 0.038, 0.040, 0.042
0.044, 0.046, 0.048, 0.050, 0.052, 0.054, 0.056, 0.058, 0.060, 0.062, 0.064, 0.068
0.070, 0.072, 0.074, 0.076, 0.078, 0.080, 0.082, 0.084, 0.086, 0.088, 0.090, 0.092
0.094, 0.096, 0.098, 0.100, 0.105, 0.110, 0.115, 0.120, 0.125, 0.130, 0.135, 0.140
0.145, 0.150, 0.155, 0.160, 0.165, 0.170, 0.175, 0.180, 0.185, 0.190, 0.195, 0.200
0.210, 0.220, 0.230, 0.240, 0.250, 0.260, 0.270, 0.280, 0.290, 0.300, 0.310, 0.320
0.330, 0.340, 0.350, 0.360, 0.370, 0.380, 0.390, 0.400, 0.410, 0.420, 0.430, 0.440
0.450, 0.460, 0.470, 0.480, 0.490, 0.500, 0.510, 0.520, 0.530, 0.540, 0.550, 0.560
0.570, 0.580, 0.590, 0.600, 0.620, 0.640, 0.660, 0.680, 0.700, 0.720, 0.740, 0.760
0.780, 0.800, 0.820, 0.840, 0.860, 0.880, 0.900, 0.920, 0.940, 0.960, 0.980, 1.000
1.050, 1.110, 1.150, 1.20, 1.25, 1.30, 1.35, 1.40, 1.45, 1.50, 1.55, 1.60, 1.65, 1.70
1.75, 1.80, 1.85, 1.90, 1.95, 2.00, 2.10, 2.20, 2.30, 2.40, 2.50, 2.60, 2.70, 2.80, 2.90
3.00, 3.10, 3.20, 3.30, 3.40, 3.50, 3.60, 3.70, 3.80, 3.90, 4.00, 4.10, 4.20, 4.30, 4.40
4.50, 4.60, 4.70, 4.80, 4.90, 5.00, 5.20, 5.40, 5.60, 5.80, 6.00, 6.20, 6.40, 6.60, 6.80
7.00, 7.20, 7.40, 7.60, 7.80, 8.00, 8.20, 8.40, 8.60, 8.80, 9.00, 9.20, 9.40, 9.60, 9.80
10.0, 10.2, 10.4, 10.6, 10.8, 11.0, 11.5, 12.0, 12.5, 13.0, 13.5, 14.0, 14.5, 15.0, 15.5
16.0, 16.5, 17.0, 17.5, 18.0, 18.5, 19.0, 19.5, 20.0, 21.0, 22.0, 23.0, 24.0, 25.0, 26.0
27.0, 28.0, 29.0, 30.0, 31.0, 32.0, 33.0, 34.0, 35.0, 36.0, 37.0, 38.0, 39.0, 40.0, 42.0
44.0, 46.0, 48.0, 50.0, 55.0, 60.0, 70.0, 80.0, 90.0, 100., 120., 140., 160., 180., 200
240, 280, 320, 360, 400, 450, 500, 550, 600, 700, 800, 900, 1000, 1500, 2000, 2500
3000, 3500, 4000, 4500, 5000, 6000, 10000, 20000, 30000, 40000, 50000, 60000
80000, 100000, 150000, 200000, 250000, 300000, 350000, 400000, 450000, 500000
600000, 700000, 800000, 900000, 1000000, 1200000, 1400000, 1600000, 1800000
2000000, 2500000.