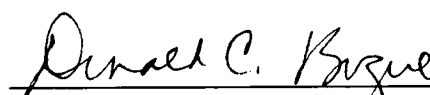
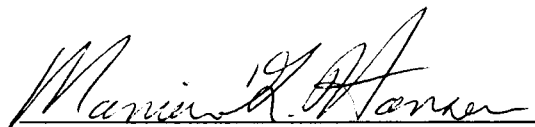


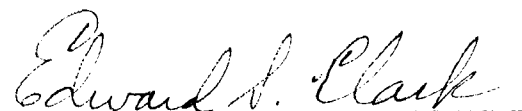
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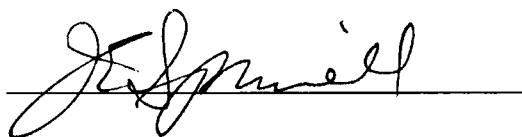
I am submitting herewith a dissertation written by Xinhua He entitled "Experiments on Time-dependent Density Changes in Amorphous Polymers and Simulation of Injection Molding." I have examined the final copy of this dissertation for form and content and recommend that it be accepted in partial fulfillment of the requirements for the degree of Doctor of Philosophy, with a major in Polymer Engineering.


Donald C. Bogue, Major Professor

We have read this dissertation
and recommend its acceptance:







Accepted for the Council:


Associate Vice Chancellor
and Dean of The Graduate School

**EXPERIMENTS ON TIME-DEPENDENT DENSITY
CHANGES IN AMORPHOUS POLYMERS
AND
SIMULATION OF INJECTION MOLDING**

A Dissertation
Presented for the
Doctor of Philosophy
Degree
The University of Tennessee, Knoxville

Xinhua He

August 1994

To Jinyi, Renke, Mom, and Dad

ACKNOWLEDGMENTS

The author wishes to express his greatest gratitude to Professor Donald C. Bogue for his invaluable guidance, discussion and encouragement during this research.

The author would like to extend his appreciation to Professor Joseph E. Spruiell, Professor Edward S. Clark and Professor Marion G. Hansen for serving on the committee.

The author would like to thank the staff of the Electronics Shop, Mr. Ted Long, Mr. Mike Neal and Mr. Steve Stiner, help in setting up the experimental system.

The author acknowledges the help of Professor C. A. Hieber and his colleagues at Cornell University, for providing the progress reports. Thanks to researchers in The Netherlands, Dr. K. M. B. Jansen, the Delft University of Technology, Dr. Reinhold Wimberger-Friedl, the Eindhoven University of Technology, for sending their Ph.D. dissertations, and Mr. G. G. J. Schennink, the Eindhoven University of Technology, for sending a report.

The author deeply appreciates the support of the Polymer Consortium and the Center for Materials Processing at the University of Tennessee, Knoxville.

A special note of thanks is given to Mr. and Mrs. Franklin and Martha Kuhlman in Wisconsin, to Mr. Benny Ban Ah Ping in Singapore for their special encouragement for me to pursue my academic goal.

Finally, the author should extend much appreciation to his loving wife Jinyi and daughter Renke for their untiring devotion. Many thanks should go to all members of the author's family for their understanding and support.

ABSTRACT

Most polymer processing operations involve a high cooling rate in which the material is cooled from a molten state into a solid state. Non-equilibrium density builds up during such a process and relaxes inhomogeneously later. These time-dependent changes also result in residual stresses. The analysis and computer simulation of various polymer processing operations are far from satisfactory because of the lack of sufficiently general theories to deal with the non-equilibrium problem. This research is part of continuing work on the residual stresses and non-isothermal rheological behavior at the University of Tennessee, Knoxville. The present study includes experiments and analysis on time-dependent density changes in amorphous polymers; and the theoretical development and simulation of injection molding.

The experimental work of the present study involved quenching bead-like polystyrene samples. The samples were subjected to air and water quenches, the average cooling rates being of the order of degrees per second by the air quench and hundreds of degree per second by the water quench. The descent of the samples in a density gradient column was measured as a function of time. Special calibration and analysis provided an estimate of the density at the end of the quench and during the subsequent aging. A rate equation and an empirical time constant equation were developed based on the data of the present work and the data of Greiner and Schwarzl. Finally, these results were used in the simulation of injection molding.

The simulation of injection molding was done on an idealized rectangular slab—taken to be homogeneous in the flat (x - y) plane, with gradients present only in the thin (z) dimension. This is only an approximation of the actual situation in injection molding, in which there are gradients in the flow direction as well. The simulation started with an imposed z -dependent temperature

distribution and an imposed time-dependent pressure distribution, simulating the end of the filling step. An imposed packing pressure is maintained by imagining that a small amount of material is added during the packing step. In the cooling step, one presumes the volume and mass to be constant. While in the post-ejection step the volume changes and the mass remains constant. The predictions are, finally, the "total stress" (pressure in the ordinary sense) as a function of time; and residual stresses and density distributions at various times.

A new concept in the theoretical framework has to do with a kind of pressure (an isotropic stress) that is used in the PVT equation—not, however, pressure in the ordinary sense. This "pressure", which is here given the symbol P , was introduced by Ko and Bogue to generalize the framework of existing constitutive theory. Temperature and hydrostatic pressure necessarily affect the volume; but certain normal loadings (for example, tensile or compressive stresses) can affect it also. The generalized isotropic stress ($-P$) can be of either sign. This becomes important in the constrained (residual stress) problem: through the thin dimension z , where the total stress σ_{zz} is a constant, one can have gradients in both P and the anisotropic stresses, often with a change of sign. These new results are discussed in detail.

Three cases were simulated in detail, approximating experimental data from groups at Cornell University, the Delft University of Technology and the Eindhoven University of Technology. In cases where "total pressure" versus time data are available, it was found that the time-dependent PVT formulation of the present work is necessary to obtain reasonable fits to the data. The predictions for residual stresses and densities cannot be tested directly because the present formulation predicts values for an undisturbed sample. In practice the sample must be cut up for testing, which releases part of the stresses. An alternate simulation was therefore done, in an attempt to simulate what was done

experimentally. This alternate simulation predicts the measured residual stresses quite well. Some features of the density distribution could be predicted qualitatively, although not quantitatively.

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CHAPTER 1

INTRODUCTION

The analysis and computer simulation of various polymer processing operations, such as injection molding and fiber spinning, are limited because of several difficulties. Actual operations are complex, involving a flow step in the molten state and a cooling step to produce a solid state. Molecular orientation in the solid state will be introduced by the prior flow. Non-equilibrium density will be introduced by the rapid cooling. The orientation and non-equilibrium density will be frozen in during the cooling and they subsequently relax inhomogeneously. Our understanding of these complex phenomena is far from satisfactory. Specifically, there is a lack of sufficiently general rheological theory to deal with non-equilibrium density changes under conditions of very rapid cooling.

Bogue and coworkers[1][2][3][4][5][6][7], at the University of Tennessee, Knoxville, have been focusing on this research area for a long period. Two important aspects, nonisothermal rheological behavior and compressible behavior have been studied.

First, the coupling of deformation response and temperature changes has been investigated by the UTK group, under the general heading of "non-isothermal rheological behavior." That is, the study puts emphasis on processes in which the stress-strain and the temperature are changed simultaneously. The experiments are usually carried out near the transition temperature and at high cooling rates.

Second, compressible effects have been included in rheological theory by coupling the stress-strain equations and the PVT or PVT-time equations. That means, for example, that when samples are constrained, stresses can be produced by temperature-induced density changes; or, when elongational stress is applied, density

changes can be produced.

Snow and Bogue[1] set down a generalized integral equation that resolved the difficulties that existing rheological equations for the rubbery and glassy states are not compatible with each other. Subsequently, Ko and Bogue[2][4] formulated an integral constitutive equation that simplifies the prior one of Snow and Bogue. Finally, Joshi and Bogue[3] have proposed a differential form of the same concepts. Those equations, in principle, allow one to deal with the non-isothermal, non-equilibrium problems. But, in practice, one needs to obtain density data first, and then uses these for testing the equations, especially at high cooling rates. There are some density data available in the literature[8][9][10][11][12] for low cooling rates, typically about 0.033 °C/sec or less. Obtaining data at high cooling rates is not easy due to several experimental difficulties[3]. There are also two reasons that the equations mentioned here are not attractive enough for practice use. One is that the equations are too complicated to be executed on computers. Another is that the equations are similar, somehow, to the classical residual stress theory, which may be closer to a free quench case rather than a constrained situation, such as injection molding, etc.

The first objective of this work was to obtain and model time-dependent density data at high cooling rates, similar to those in injection molding. The second objective was to develop a complete theoretical framework to describe PVT changes and density-induced residual stresses in a flat rectangular slab, which simulates all post-filling steps in injection molding, that is, packing, cooling and post-ejection. The third objective was to execute the above equations on the computer and to compare the results for pressure-decrease, residual stresses and density distribution with literature data from groups at Cornell University[86][87][88], the Delft University of Technology[81] and the Eindhoven University of Technology[82].

CHAPTER 2

BACKGROUND

A review of certain basic subjects is needed here. The first subject discussed is linear elasticity theory for equilibrium stress-strain response and compressibility. The second subject is compressible viscoelastic theory in integral formulation and differential formulation. Rate equations and free volume theories will be the third part, which includes temperature, pressure effects and their time dependence. The final part has to do with residual stresses in injection molded articles, which will cover measurement techniques, classical theories and analyses of residual stresses.

§2.1. Linear Elasticity Theory

Linear elasticity theory is employed to describe the mechanical behavior of polymers with solid-like properties. Considering a completely isotropic case, the equations are given by

$$\bar{\sigma} = \lambda (\text{tr} \bar{\epsilon}) \bar{\delta} + 2G \bar{\epsilon} \quad (2.1)$$

$$(\text{tr} \bar{\epsilon}) = \frac{\Delta V}{V} \quad (2.2)$$

where $\bar{\delta}$ is a unit tensor or Kronecker delta, $\bar{\sigma}$ is the total stress tensor, $\bar{\epsilon}$ is the extra strain tensor, $(\text{tr} \bar{\epsilon})$ is related to volume changes, and λ and G are Lamé constants[13][14]. From these equations, one can obtain the following isotropic results[14][15][16],

$$E = \frac{G(3\lambda + 2G)}{\lambda + G} \quad (2.3)$$

or,

$$E = 2G(1 + \nu) \quad (2.4)$$

$$E = 3B(1-2\nu) \quad (2.5)$$

where E is the Young's modulus, B is the bulk modulus, and ν is the Poisson's ratio.

There are some alternative forms of Eq.(2.1)[14][15]. In the rubber-like case, $(\text{tr}\bar{\epsilon}) \rightarrow 0$, $\lambda \rightarrow \infty$, by an undetermined scale p , one has

$$\bar{\sigma} = -p\bar{\delta} + 2G\bar{\epsilon} \quad (2.6)$$

For cases where thermal stresses exist, one has

$$\bar{\sigma} = [\lambda(\text{tr}\bar{\epsilon}) - \bar{\alpha} \left(\frac{2}{3} G + \lambda \right) (T - T_0)] \bar{\delta} + 2G\bar{\epsilon} \quad (2.7)$$

where $\bar{\alpha}$ is the thermal expansion coefficient, T is the instantaneous temperature, T_0 is the initial temperature (reference temperature). Of course, linear elasticity theory is restricted to small strains, without time effects.

Nonlinear elasticity theory is used to deal with large deformation (strain) problems, but the theory for the deformation assumes incompressibility. This assumption is in contradiction to the linear cases discussed above. That is, the linear and nonlinear theories are not consistent. Recent work which eliminates the inconsistency will now be discussed.

§2.2. Compressible Viscoelasticity Theories

§2.2.1. Integral Compressible Models

Volume effects have to be accounted for in the glassy state, such as by using linear elasticity theory. However, in the rubbery

state, amorphous polymers are considered to be incompressible. This is the assumption made in the classical viscoelastic theories. Thus, the theories for rubbery state and glassy state are not compatible with each other.

In earlier work, Snow and Bogue set down a generalized integral model, which accounts for compressible effects in both the rubbery and glassy states. The rheological equation for stress is expressed in two terms, one having to deal with isotropic volume changes and the other due to anisotropic deformations[1][5].

The generalized integral model is applicable to describe both the volume and orientation effects. Also, it could be reduced to several existing theories, in particular:

- (1) linear elasticity theory,
- (2) incompressible viscoelasticity theory,
- (3) an equilibrium PVT equation, and
- (4) a volume rate equation.

However, Snow and Bogue's equations are so complicated that they cannot be used except in a few simple cases.

Ko and Bogue[2][4][6] presented a restatement of the Snow-Bogue integral model in a more tractable and slightly modified form. The key idea in the Ko-Bogue formulation is to introduce an isotropic negative stress P , which is the hydrostatic pressure in isotropic deformation, but in general depends on the anisotropic stresses as well.

The Ko-Bogue formulation consists of three simultaneous equations, a generalized PVT equation, a generalized anisotropic stress equation, and an equation of continuity, as follows:

$$\frac{D(\theta + \phi_f)}{Dt} = - \frac{\Delta \theta}{\tau(t)} \quad (2.8)$$

$$\sigma_{ij} = -p\delta_{ij} + \int_{-\infty}^t \left[\frac{G(t')}{\tau_G(t')} \exp\left[-\int_{t'}^t \frac{dt''}{\tau_G(t'')}\right] (c_{ij}^{-1})^* \right] dt' \quad (2.9)$$

$$\sqrt{\det c_{ij}^{-1}} = \frac{V(t)}{V(t')} \quad (2.10)$$

where

$$\frac{D\bullet}{Dt} \equiv \frac{\partial\bullet}{\partial t} + v_k \frac{\partial\bullet}{\partial x_k} \quad (2.11)$$

$$\theta(t) = \frac{p(t)}{\lambda^*(t)} + \frac{V(t)}{V_0} - \alpha(t)T(t) \quad (2.12)$$

$$\begin{aligned} \Delta\theta(t) &= \theta(t) - \theta(0) \\ &= \frac{p(t) - P_0}{\bar{\lambda}^*} + \frac{V(t) - V_0}{V_0} - \bar{\alpha}(t) [T(t) - T_0] \end{aligned} \quad (2.13)$$

$$\phi_f(t) = \Delta\alpha(t) [T(t) - T_{ge}] - \Delta\kappa(t) [p(t) - P_0] \quad (2.14)$$

$$(c_{ij}^{-1})^* = c_{ij}^{-1} - \delta_{ij} - \frac{2}{3} \frac{\Delta V}{V(t')} \quad (2.15)$$

where t is the instantaneous time, t' and t'' denote the past times, V is the specific volume, $\tau(\bullet)$ is the relaxation time associated with local motion of polymer molecules, $\tau_G(\bullet)$ is the relaxation time associated with long-range motion of polymer molecules, $\bar{\lambda}^*$ is a properly averaged modulus, $\lambda^*(\bullet)$ is the bulk modulus, $\bar{\alpha}$ is a properly averaged coefficient of thermal expansion, ϕ_f is the driving force term for change of pVT state, (c_{ij}^{-1}) is the conventional Finger strain tensor, $(c_{ij}^{-1})^*$ is the normalized Finger strain tensor, σ_{ij} is the total stress, p is the negative scale stress, θ is a variable which characterizes the pVT state, $\Delta\theta$ is a measurement of the extent of nonequilibrium among the variables, p , V and T (two of which are

independent). The most important term in the formulation is the time constant $\tau(t)$ [4][6]. The time constant depends on time because the variables, p , V and T depend on the cooling rates and on the nonequilibrium volume. All these effects can be dealt with by some suitable shift factors applying to the reference time constant, τ_0 . It will be discussed individually later. The form given above, the Ko-Bogue formulation, is a one element equation. The more general form was given in the papers[2][4].

§2.2.2. Differential Compressible Model

Both of the Snow-Bogue and Ko-Bogue formulations discussed above are integral models. The cases they treated are isotropic problems, which means that the temperature and deformation profiles are homogenous throughout the parts. With those special cases, then, they dealt with the energy and force equations there with much simplification. Finally, the integral models reviewed in the previous section were put in an attractive form. But even so, they are still difficult for use in a practical program. A set of equations in differential form is desired and will expedite executing them by computer. This work was started by Joshi and Bogue[3][7]. By studying a similar homogenous case, they have presented a differential compressible model using the same concepts, which mainly consist of a generalized PVT equation, a continuity equation and a generalized anisotropic stress equation. The generalized PVT equation is the same as the one in the Ko-Bogue formulation, which reads as

$$\frac{D(\theta+\phi_f)}{Dt} = - \frac{\Delta\theta}{\tau(t)} \quad (2.8)$$

where the various symbols have been defined previously. The generalized anisotropic stress equation is now stated as

$$\sigma'_{ij} + \tau_G(t) \frac{\delta \sigma'_{ij}}{\delta t} = G(t) \tau_G(t) d_{ij}^* \quad (2.16)$$

where

$$\sigma_{ij} = -p\delta_{ij} + \sigma'_{ij} \quad (2.17)$$

$$d_{ij}^* = \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} - \frac{2}{3} \frac{\partial v_k}{\partial x_k} \delta_{ij} \quad (2.18)$$

where σ'_{ij} is the extra stresses, $\frac{\delta \sigma'_{ij}}{\delta t}$ is a contravariant derivative, (the so-called "upper" convected derivative), and d_{ij}^* is a normalized deformation rate tensor, normalized so as to remove the deformation due to volume changes only. Both $G(t)$ and $\tau_G(t)$ are functions of temperature (and thus of time). The continuity equation is given by [56],

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho v_i)}{\partial x_i} = 0 \quad (2.19)$$

Joshi and Bogue have numerically confirmed that these equations are equivalent to the Ko-Bogue integral type equations in a homogenous analysis [7].

In a general problem, one needs a force balance equation and energy equation (as shown, for example, in [56].) But, when one deals with a simple problem, most terms in both of these equations will not be presented. That means these two equations can be simplified and may be solved separately. Then, one has a set of simultaneous equations, that is, the generalized PVT equation (Eq.2.8), the generalized anisotropic stress equation (Eq.2.16) and the continuity equation (Eq.2.19), as mentioned above [1][2][3][4][5][6][7]. Also, the equations can be given in multiple element form [3].

§2.3. Free Volume Concepts and Rate Equations

Based on the free volume concept, many rate-dependent equations have been proposed, as will be reviewed below.

A free volume concept based on liquid theory was first introduced by Fox and Flory[25]. Turnbull and Cohen[27][61] proposed that the free volume corresponds to the excess volume which can be redistributed without any changes in energy[13]. Similarly, Simha and Boyer[28] defined a fraction of free volume related to glass transition temperature. Williams, Landel and Ferry[26] presented a frequently used equation, (the WLF equation), which is also based on a free volume concept.

There are several kinds of volume rate equations based on free volume concepts[18][19][20][21][22][23][24]. Reviews have been given by several authors[9][18][20][29]. Under the conditions of constant pressure, Tool[30], Saito et al[31], Davies and Jones[32], Goldbach and Rehage[33][34], and Kovacs and coworkers[18][20][21] have used the first-order rate equation,

$$\frac{d(V-V_{\infty})}{dt} = -\frac{V-V_{\infty}}{\tau(t)} \quad (2.20)$$

where V_{∞} is the equilibrium volume at infinite time. We now introduce a symbol δ , the recoverable free volume, as used by Kovacs and others,

$$\delta = \frac{V-V_{\infty}}{V_{\infty}} \quad (2.21)$$

which yields the rate equation including temperature effects.

$$\frac{d\delta}{dt} = -\frac{\delta}{\tau(t)} - \Delta\alpha \frac{dT}{dt} \quad (2.22)$$

$$\tau(t) = \tau(T, \delta) = \tau_0 a_T a_\delta \quad (2.23)$$

They later generalized these equations to include pressure effects as well[18][20][21]

$$\frac{d\delta}{dt} = -\frac{\delta}{\tau(t)} - \Delta\alpha \frac{dT}{dt} + \Delta\kappa \frac{dP}{dt} \quad (2.24)$$

$$\tau(t) = \tau(T, P, \delta) = \tau_0 a_T a_P a_\delta \quad (2.25)$$

where τ_0 is the initial relaxation time at T_0 , P_0 and δ_0 ; a_T , a_P and a_δ are the shift factors responding to temperature changes, pressure changes, and non-equilibrium volume, respectively.

Turnbull and Cohen[27] considered the free volume as a distribution of holes of various sizes in the continuum. This is apparently the motivation for the multi-parameter models that have been developed by Kovacs and coworkers[18][35] and others[36][37].

The cooling rates in the work mentioned above are typically in the range of several degrees per minute or lower. In practice, however, most polymer processes involve very high cooling rates, for example, tens of degree per second or hundreds of degree per second in injection molding, or thousands of degree per second in melt spinning. These high cooling rates introduce nonequilibrium volume and nonequilibrium orientation, which affect the mechanical properties of the parts as well as subsequent aging. Also, polymer processing operations sometimes involve large changes in pressure. Although the problem of high cooling rates need a great deal more study, the question of combining the PVT-time effects and stress effects has been dealt with by Ko and Bogue[2][4]. Looking at the

PVT part of generalized equations they presented, Eq.2.8 to Eq.2.14, the special equations for the compressibility effects are

$$\frac{dV}{dt} = -\frac{V-V_e}{\tau(t)} + V_0 \alpha_g \frac{dT}{dt} - V_0 \kappa_g \frac{dp}{dt} \quad (2.26)$$

$$V_e = V_0 [1 - \bar{\alpha}\Delta T - \bar{\kappa}p] \quad (2.27)$$

where V_0 is the specific volume at T_0 and P_0 , V_e is the equilibrium volume, and $\Delta T = (T_0 - T)$. One may note that Eq.2.26 and Eq.2.27 are similar to Eq.2.22 and Eq.2.23, and Eq.2.24 and Eq.2.25, except that Eq.2.26 and Eq.2.27 are linearized around V_0 instead of V_∞ .

§2.4. Residual Stresses in Injection Molded Parts

§2.4.1. Nature of Residual Stresses and Their Measurement

Stresses due to molecular orientation and their relaxation are mainly dependent on chemical structure, rheological properties, geometry and processing conditions. Usually, the stresses due to the molecular orientation should be referred to as residual orientation rather than residual stresses. These are not taken into account in this work. Stresses due to volume changes are related to the viscoelastic behavior of the polymer, which are time-dependent. This research work emphasizes these stresses. One needs to discuss some experimental methods for the measurement of residual stresses before discussing these stresses in detail.

Such stresses are macroscopically observable stresses due to nonuniform cooling and volume changes. These stresses are not easily measured, although some methods have been developed[70]. The techniques, many of which were developed in the metallurgical area, consist of such methods as hole-drilling, in which one observes the change of shape and dimension of the hole; a layer-removal

method which measures the bending of the remaining sample; and birefringence method which has been applied here, at the University of Tennessee by Wust and Bogue[54][62]. The disadvantage of the birefringence is that the connection between the birefringence method and residual stresses is very complicated during rapid quenching. The most reliable method, but a very complicated one, is the layer-removal technique, which involves layer-by-layer removal of polymer samples followed by observation of the bending of the remaining sample. This technique was introduced by Treuting and Read[42], and has been used in recent years. More detail can be found elsewhere[10][11][43][57][63][64][65][66]. Classical residual stress theories and certain more recent work will now be reviewed.

§2.4.2. Classical Residual Stress Theories

When polymeric parts are subjected to an unconstrained quench at high rates, the volume-induced residual stresses build up significantly. Theories for the calculation of residual stresses in a free quenched slab were initially presented by Indenbom[40][41], and later by Aggarwala and Saibel (AS)[39]. These simplified theories were generalized by Lee, Rogers and Woo (LRW)[34]. A basic assumption for all these theories is that the PVT equation is time-independent. The modulus, however, is time-dependent in the LRW theory, which is not true in the other cases. The central ideas of the theories will now be summarized.

Consider an amorphous polymeric slab, which is thinner in the z-direction and of infinite extent in the x-direction and y-direction. The slab has its boundary conditions,

$$0 = \int_0^{H_z} \sigma(z,t) dz \quad (2.28)$$

where

$$\sigma(z,t) = \sigma_{xx} = \sigma_{yy} \quad (2.29)$$

where H_z is the half thickness in the z -direction, the thinnest one.

The boundary conditions imply that

(1) both ends of the slab in the x - and y -directions are "solidified cages", that is the ends are imagined to be solid and to move uniformly;

(2) all imagined layers have uniform lengths, $L_x(t)$ and $L_y(t)$, in two long-dimension directions at time t ; and

(3) the lateral expansion in the z -direction is free, i.e., $\sigma_{zz} = 0$.

By assuming linear elasticity theory and an equilibrium PVT relationship, one can relate the trace of stress to the volume change and the temperature changes. By these means, the LRW theory gives the strain, $\epsilon_z(z,t)$, and the stresses, $\sigma_{xx}(z,t)$ [$=\sigma_{yy}(z,t)$], as follows:

$$\epsilon_z(z,t) = \frac{2\sigma_{xx}(z,t)}{3B} - 2\epsilon_x(t) + 3\alpha[\Delta T(z,t)] \quad (2.30)$$

$$\sigma_{xx}(z,t) = \int_0^t 2G(t-t') \frac{\partial[\epsilon_x(t') - \alpha T(z,t')]}{\partial t'} dt' \quad (2.31)$$

where

$$\Delta T(z,t) = T(z,t) - T(z,0) \quad (2.32)$$

where $G(t-t')$ is a time-dependent modulus function. This function in the LRW theory is continuous. In the earlier special case of Aggarwala and Saibel (AS), the analogous function is discontinuous, that is,

$$M(\Delta\zeta') = \begin{cases} 0 & \text{at } T > T_g \\ M_c & \text{at } T < T_g \end{cases} \quad (2.33)$$

where M_c is the characteristic modulus in the glassy state, and $\Delta\zeta'$ is the reduced time. Thus the AS model can be expressed as

$$\sigma_{xx}(z,t) = \int_{t(T_g)}^t 3M_c \frac{\partial[\varepsilon_x(t') - \alpha T(z,t')]}{\partial t'} dt' \quad (2.34)$$

A similar simplification was made by Indenbom[40][41] who considered the total strain being composed of three components, a time-dependent strain, i.e., a temperature-dependent strain, an elastic strain, and a "plastic" strain. The assumptions are that the "plastic" strain is time-dependent at $T < T_g$, that the time-dependent strain is position-dependent, and that the elastic strain is only for that $T \leq T_g$ or $t \geq t(T_g)$. Indenbom's equation is a special case of the AS model.

§2.4.3. Measurement and Analysis of Residual Stresses

Many research groups have focused on the measurement and analysis of residual stresses. Reviews have been given by Isayev[43] and Huilier[58] et al. A brief summary will be given here.

Struik[29][67][76] considered the various effects in molding products, as previously discussed. Struik generalized the AS theory to a complicated geometry, but like the AS theory, the characteristic coefficients (such as Young's modulus, bulk modulus, heat capacity, etc.) are constants, although they change at T_g : that is, they change discontinuously from rubbery values to glassy values.

Related studies of a similar sort have been reported by Greener[12], Siegmann, et al.[10][63][68][69], Isayev and Hariharan[11][43][57]. For example, Isayev and Hariharan applied a first-order rate equation for specific volume aging and obtained a

numerical simulation for the density recovery.

J. R. White and coworkers[64][65][66][71][72][73][74][75] have worked in this field for a long time. Their work has mostly focused on the properties of materials which are semicrystalline, or are filled polymers. They pointed out that the physical property changes are at least partly reversible, with rapid recovery occurring within the first twenty-four hours after returning to room temperature. The changes are not homogeneous. Also, it is not possible to correlate fatigue fracture behavior simply with the residual stress and/or the birefringence of an amorphous polymer part, such as in a PC molding. In some complicated way the mechanical properties depend on the thermal history of the material. For example, Young's modulus varies with depth, although it does not produce very large changes in the profile of residual stresses. In fact, the residual stress levels decrease with increasing filler and they change in a complicated way with crystallinity and environmental conditions.

Ko[6] developed a simulation which more closely follows the physical picture of what happens in an injection molding part. He imagined a slab made up of many thin layers, all of which have the same lengths in the two long-dimensions. The layers expand and constrict freely in the short-dimension. However, each layer constricts differently because each layer has a different thermal history. This situation causes stresses to be developed in the overall sample. Equations are presented in a general manner. Then, for an initial analysis a simple case was studied. In particular, he imagined, similar to Aggarwala and Saibel, that the characteristic response is either fluid-like, (i.e., no memory), or solid-like, (i.e., full memory). But unlike the AS and other prior theories, Ko introduced the notion that the volume changes depend on temperature and time. In what he called the equilibrium case, the volume changes depend on temperature only. In the nonequilibrium case, the volume changes are dependent on time and temperature. Ko stated the equations, but the complicated analysis was not completed.

Recently, Jansen[81] investigated the effects of both thin insulation foil and active heating elements on the frozen-in orientation and residual stresses, that is, the temperature history effects. The relationship of the polymer flow and the heat transfer is derived for the temperature profiles during injection molding. Then, the thermal history effects on both of the orientation relaxation and residual stresses of injection molded parts were discussed. The pressure, temperature and residual stresses of the parts were measured experimentally, using the layer removal technique for the residual stresses. The discussion of residual stress is put in terms of Struik's cooling stress model.

Schennink[82] studied the dimensional stability of injection molded parts, (polystyrene, polycarbonate, etc.,) in terms of volume relaxation and orientation/frozen-in strain. The equation of state (the PVT equation) is based on a thermodynamic equilibrium theory, the stochastic Holey-Huggins theory. Dilatometric and density gradient column (DGC) experiments were employed to determine the density distribution profile. The study shows that cooling rate induces densification and that volume relaxation is one of the important facts for the dimensional stability of injection molded parts. The study of the recovery of frozen-in strains was based on the C-FLOW program, which uses the same equilibrium assumption[89][94].

Huilier[58] has comprehensively reviewed the modeling problem of injection molding. The general problem involving the effects of thermal and pressure history on the volume and stress equations are extremely complicated. The nonhomogeneous nature of the temperature and pressure fields is also a complication. In the existing literature on residual stresses, mostly the sample is a freely quenched one. But in injection molding, the sample is constrained during packing and cooling steps and is free during the post-ejection step. This basic difference means, then, that more general equations must be developed.

CHAPTER 3

TIME-DEPENDENT DENSITY CHANGES: EXPERIMENTS AND ANALYSIS

In continuing work at the University of Tennessee, Knoxville, Bogue and coworkers[1][2][3][4][5][6][7] have stated equations for time-dependent compressible effects in amorphous polymers. But a basic difficulty remains—that is, one needs rate-dependent density data at high cooling rates to simulate actual polymer processes such as injection molding. One objective of the present work was to measure density data under rapid quench conditions, or at least, to infer them indirectly. A secondary objective was to analyze the experimental work to obtain some parameters necessary for describing these density changes as well as for developing a rate equation. A final one was to form a rate equation, which would subsequently be used in the analysis of a problem of practical interest, the injection molding problem. This work will now be presented in detail.

§3.1. Experimental Procedures

Most polymer processes involve rapid cooling from a molten state to a solid state. In practice, polymer processing operations, such as injection molding and fiber spinning, cover a wide range of cooling rates. In injection molding, for example, the cooling rates can vary from tens to hundreds of degree per second, or even higher, to thousands of degree per second in fiber spinning. The present experiments, which emphasize rapid cooling rates, involved determining the cooling rates quantitatively, measuring the density of the samples at the end of quench and density changes during aging. Rate-dependent volume-temperature data have typically been obtained from dilatometry experiments, from which the cooling rates are very low: 120 [°C/hr] (0.033 [°C/sec]) or less[8]. A major objective of the work was to obtain such data at much higher cooling

rates. It is very difficult to measure the density and its changes directly during quenching and aging with high quench rates. There are some experimental difficulties in carrying out the measurement of the quench rates and volume changes. The first one is the heat transfer effect. If a sample used for the measurement is large enough to measure its volume and the mass directly, there will be significant thermal inhomogeneities in the sample. This will result in a nonuniform density. The second one is the effect of response time. Since the cooling rates are so high, the total quench time is very short. That requires that the equipment and operating procedure be responsive to the temperature changes. The third one is the fast aging of the samples after rapid quench. If one quenches a sample at high rates, its density will change very fast in a short period after the end of quench (minutes or even seconds) due to the large amount of nonequilibrium volume. It is not easy to measure the density of the sample and its changes in so short a time. The present experiments dealt with these difficulties only indirectly. The density or specific volume changes were measured indirectly by quenching samples under controlled thermal conditions and measuring the resulting densities in a density gradient column (DGC). This work will now be described below.

§3.1.1. Materials, Samples and Equipment Set-up

A commercial polystyrene (PS), Shell TC 3-30 from the Shell Chemical Company, was employed in this work. The material has been used in many long-term studies here at the University of Tennessee. The molecular weights are $M_w=2.8 \times 10^5$ and $M_n=6.1 \times 10^4$, which give $M_w/M_n=4.6$. The well-aged density is $\rho_\infty=1.05$ [g/cm³]. The samples used for the measurement of density changes were that of commercial beads in their original states, which have been stored at room temperature for more than ten years. The pellets are in the shape of small cylinders with dimensions $D \approx L \approx 1.1$ [mm]. The rheological behavior of the polymer under wide ranges of

temperature and time scales have been measured extensively[1][44][45][46][47][48][49][50].

The samples used for the measurement of quench rates were imbedded with small thermocouples (TC), IRCO-005 (diameter in 0.005 [inch], or 0.127 [mm].) These simulated samples were used in parallel with the actual PS pellets. The total thickness of the thermocouple imbedded in a polystyrene "sandwich" was in the range of 0.6 to 1.0 [mm]. The size was chosen to simulate the actual PS pellets. There is undoubtedly a temperature gradient in the pellets at high quench rates, but the metal thermocouple embedded in the center provides a kind of average temperature profile.

Two quenching processes were carried out in the experiments: quenching by air at 23 °C and by water at 10 °C. All experiments were done under atmospheric pressure.

A schematic diagram of the experimental system is shown in Figure 3.1-1, which include samples for both of the temperature measurements and quench processes. The system consists of an IBM-PC computer, an amplifier, a printer, a hot stage system, a PS covered thermocouple, and a water quench bath. The IBM-PC computer controls experimental procedure by taking data automatically and displaying the results. The amplifier connects the thermocouple to the IBM-PC and transfers the output signal of the TC to the input of the computer. The hot stage system provides heating conditions as needed.

§3.1.2. Determination of Quenching Rates

The quench rates were determined in the following method. First, the samples, consisting of thermocouples covered by PS, were heated to 120 °C by the hot stage system at rates of 5 or 10 [°C/min], and held at that temperature for 10 to 15 minutes to allow equilibrium. Then the samples were quenched by air at 23 °C, or by

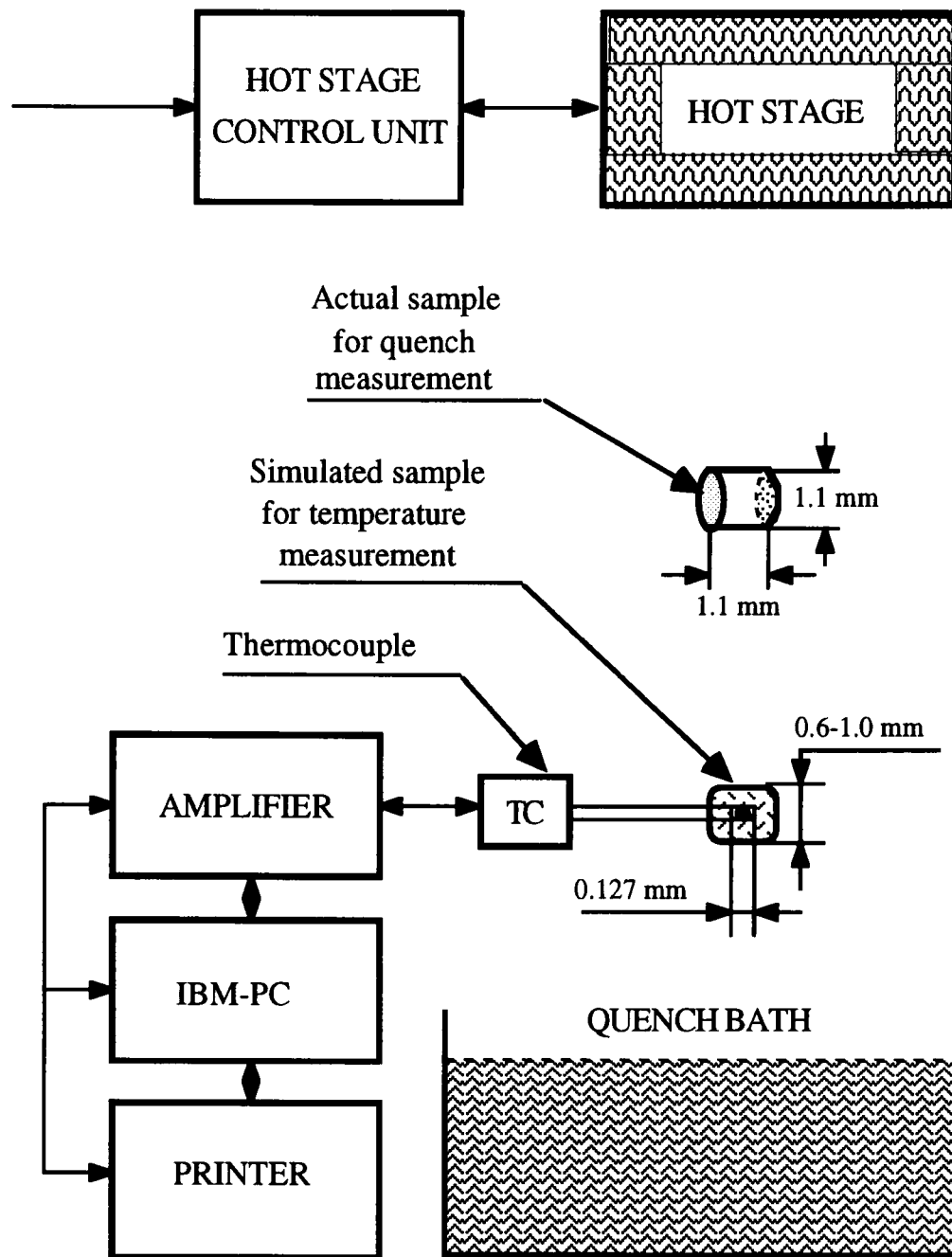


Figure 3.1-1 Experimental set-up for quenching measurements

water at 10 °C. The data taken are temperature versus time, as shown in Figure 3.1-2, presents the thermal histories of samples. These data were later fitted by smoothing equations. The experiments show that the air quench rates are in the range of several degrees per second and the water quench rates are in the range of hundreds of degree per second.

§3.1.3. Measurement of Density Changes

The starting point for the density measurements was the method prescribed by the Standard of American Society for Testing and Materials, (ASTM, D1343-86). Unfortunately, such measurements do not account for time lags. With a special hydrodynamic calibration and analysis, one can overcome this difficulty. The experimental procedures are described below. The analysis will be given in the following section.

There were two main experimental procedures to make the measurements of density changes. First, well-aged samples were used for the calibration. Then the samples, which were exactly the ones used in the calibration step, were subjected to heating, quenching, and free aging. At the end of the quench, pellet-like PS samples were put into the DGC. The aging and settling processes were measured. Details and results are reported below.

An ethylene glycol-water DGC was made for the measurement of the density of the samples. The ranges of the DGC were from 1.020 [g/cm³] to 1.065 [g/cm³][51][52][54][77][78]. The DGC was run at the room temperature (23 °C).

For calibration, well-aged PS beads were directly put into the DGC before they were subjected to heating and quenching. The descent in the DGC as a function of time was measured. One takes the readings continually until the samples reach their equilibrium positions. Usually this step will take more than twenty-four hours.

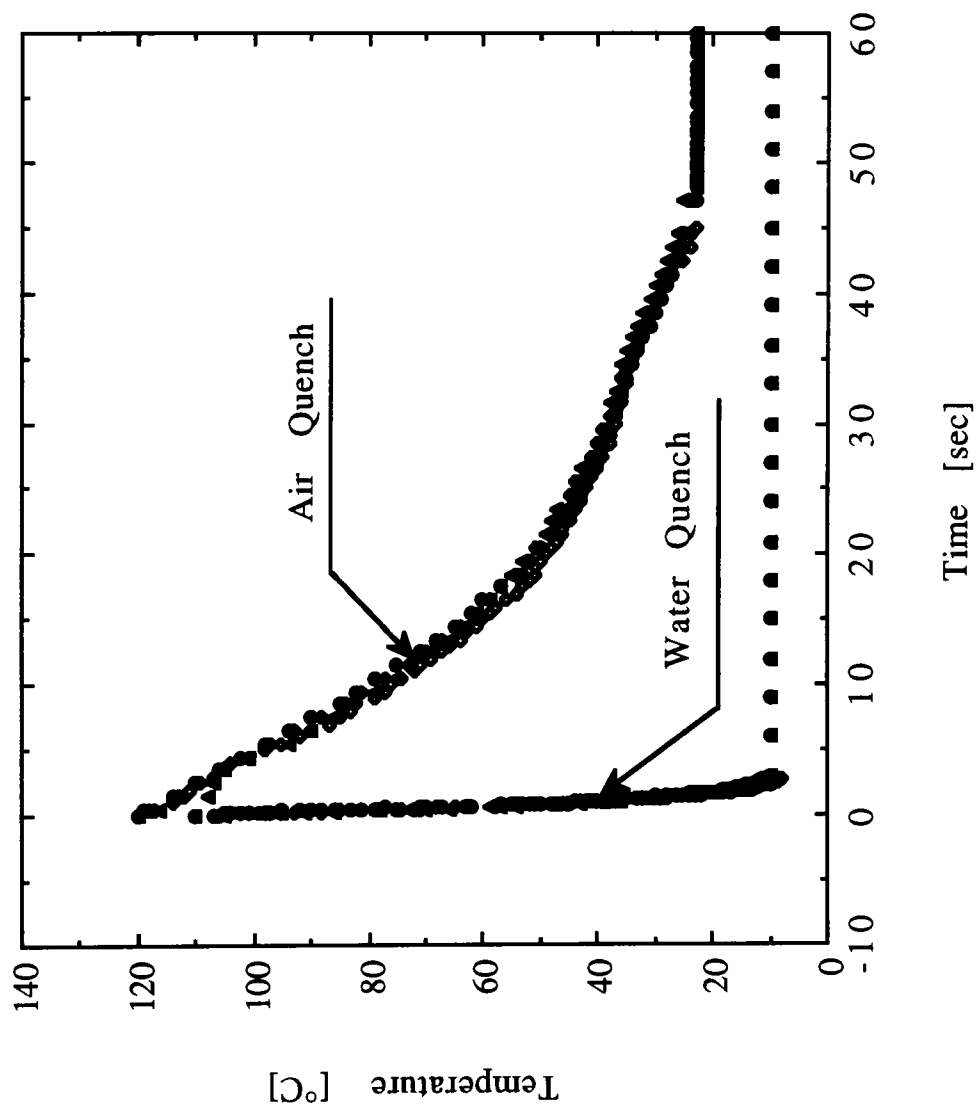


Figure 3.1-2 Temperature profiles of the bead-like samples during quenching

After the calibration step was done, the samples were removed from the DGC and used for the quench measurements. When measuring the quenching and aging processes, the thermal treating procedures which were employed in the quench rate measurements were repeated, except that the samples used here were the same beads used in the calibration step. Because the details are important, the steps of thermal treating procedures are repeated here. First, the samples were heated up to 120 °C by the hot stage system (with rates of 5 or 10 [°C/min]), and held at that temperature for 10 to 15 minutes to allow equilibrium; then they were quenched by air at 23 °C, or by water at 10 °C. At the end of the quench, the samples were immediately put into the DGC. The descent as a function of time was measured again. Figure 3.1-3 is the plot of these data.

§3.2. Analysis of Experimental Work

When a sample, either a well-aged or a quenched one, is descending in the DGC, it must satisfy a force balance equation:

$$F_g + F_d(z) + F_b(z) = M_s \frac{d^2 z}{dt^2} \quad (3.1)$$

where

$$F_g = M_s g = \text{constant} \quad (3.2)$$

$$F_d(z) = - 6 \pi \mu_s R_s(z) \frac{dz}{dt} \quad (3.3)$$

$$F_b(z) = - \frac{M_s}{\rho_s(z)} \rho_f(z) g \quad (3.4)$$

where $z=f(t)$ is the position of a bead in the DGC at time t as measured from the top, F_g is the gravity force, $F_d(z)$ is the drag force by Stokes' law, $F_b(z)$ is the buoyancy force. Positive forces are downward-acting forces in the positive z -direction. M_s is the mass of

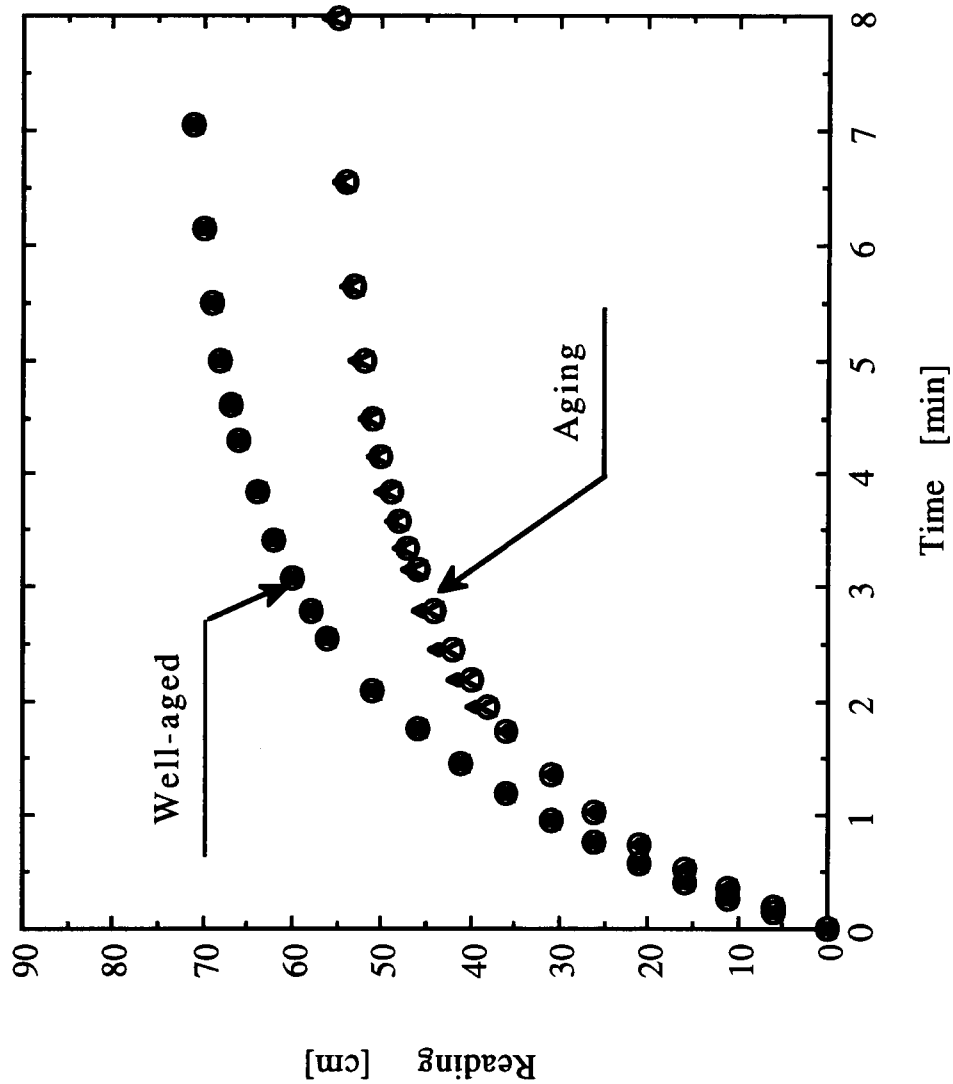


Figure 3.1-3 Vertical position of the samples in the DGC

the sample, g is the acceleration due to gravity, $\rho_f(z)$ is the fluid density at the position z , $\rho_s(z)$ is the sample's density, $R_s(z)$ is the effective radius of the sample, and $\mu_s(z)$ is an effective local viscosity.

Stokes' equation involves the infinite fluid and creeping flow. In the present case, wall effects on the settling of a sample in the DGC have to be carefully considered[51][52][53][54][55][77][78]. There are some kinds of equations for dealing with the wall effects. A common one is the so-called Faxen equation[53][55][78],

$$\mu_s(z) = \frac{\mu_0(z)}{1 - a_1\gamma + a_3\gamma^3 - a_5\gamma^5} \quad (3.5)$$

where

$$\gamma = \frac{R_s(z)}{R_c} \quad (3.6)$$

where γ is the radius ratio, $\mu_0(z)$ is the fluid viscosity for very small Reynolds' number, $N_{Re} \rightarrow 0$; a_1 , a_3 and a_5 are constants, and R_c is the inside radius of the DGC tube. If $\gamma \ll 1$, one has

$$\mu_s(z) = \frac{\mu_0(z)}{1 - a_1\gamma} \quad (3.7)$$

For calibration with a well-aged sample, its density is a constant, that is $\rho_s(t) = \rho_\infty$. So that the effective viscosity, $\mu_s(z)$, and the effective radius of the sample, $R_s(z)$, can be determined by Eq.3.1 to Eq.3.4, Eq.3.6 and Eq.3.7. That is,

$$R_s(z) = \frac{M_s R_c \left\{ g[\rho_\infty - \rho_f(z)] - \rho_\infty \frac{d^2 z}{dt^2} \right\}}{6\pi \rho_\infty R_c \mu_0(z) \frac{dz}{dt} + a_1 M_s \left\{ g[\rho_\infty - \rho_f(z)] - \rho_\infty \frac{d^2 z}{dt^2} \right\}} \quad (3.8)$$

or,

$$\mu_s(z) = \frac{6\pi\rho_\infty R_c \mu_o(z) \frac{dz}{dt} + a_1 M_s \left\{ g[\rho_\infty - \rho_f(z)] - \rho_\infty \frac{d^2 z}{dt^2} \right\}}{6\pi\rho_\infty R_c \frac{dz}{dt}} \quad (3.9)$$

These calibration results were used in the analysis of aging and settling processes. Then, the density of the sample aging in the DGC can be determined by

$$\rho_s(t) \equiv \rho_s(z(t)) = \frac{M_s g \rho_f(z) [a_1 R_s(z) - R_c]}{M_s \left[g - \frac{d^2 z}{dt^2} \right] [a_1 R_s(z) - R_c] + 6\pi R_c \mu_o(z) \frac{dz}{dt}} \quad (3.10)$$

Figure 3.2-1 shows the density calculated by Eq.3.10. One can also extrapolate it to the "position zero" or "time zero" to estimate the densities there, i.e., at the end of the quench, which is the beginning of the DGC experiment.

§3.3. Development of Rate Equations

A model for rate-dependent volume changes using a wide range of cooling rates is needed for the rheological and residual stress analysis. But rate-dependent volume data at high quench rates are lacking in the present literature. The experiments described above have provided the data, but analysis of them is necessary to obtain a rate equation. This analysis is presented below.

Since the experiments are isobaric free quench ones, the Ko-Bogue rate equation, Eq.2.26, reduces to the first-order rate equation

$$\frac{dV}{dt} = - \frac{V - V_e}{\tau(t)} + V_0 a_g \frac{dT}{dt} \quad (3.11)$$

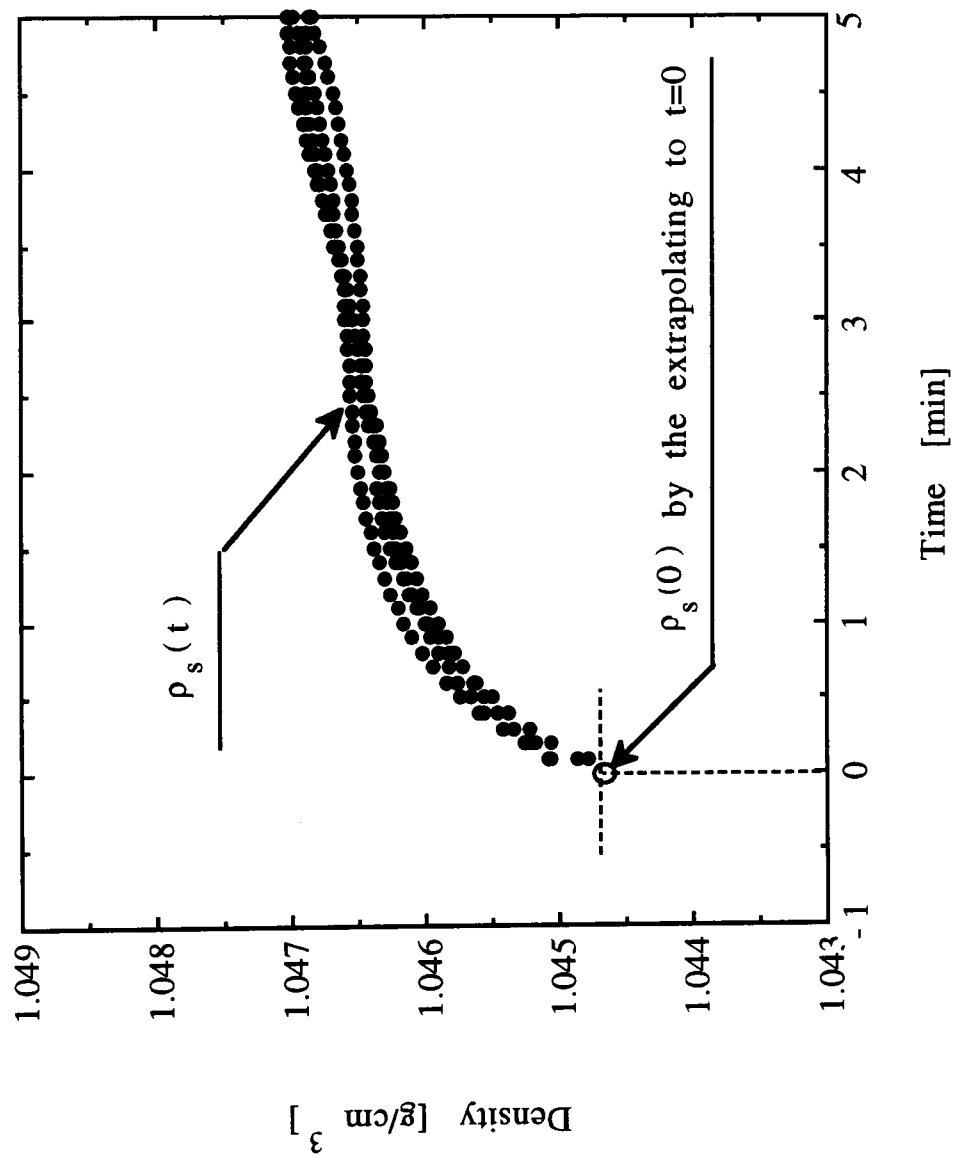


Figure 3.2-1 Density of the samples aging in the DGC, calculated by Eq. 3.10

where

$$V_e = V_0[1 - \alpha_r(T_0 - T)] \quad (T > T_{ge}) \quad (3.12)$$

$$V_e = V_0[1 - \alpha_r(T_0 - T_{ge}) - \alpha_g(T_{ge} - T)] \quad (T < T_{ge}) \quad (3.13)$$

The symbols were defined previously. The equation, Eq.3.11 can be employed to deal with the volume changes during quench and subsequent aging. However, the equation is not applicable until the time constant, $\tau(t)$ is determined. Therefore, the time constant problem must be solved first.

Using density, instead of specific volume, the rate equation can be rewritten, at the conditions of constant temperature and constant pressure, as follows:

$$\frac{d}{dt} \left[\frac{\rho_\infty - \rho_s(t)}{\rho_s(t)} \right] = - \frac{\rho_\infty - \rho_s(t)}{\rho_s(t)\tau(t)} \quad (3.14)$$

Integrating Eq.3.14 from 0 to t, one gets

$$\rho_s(t) = \frac{\rho_\infty \rho_s(0)}{\rho_s(0) + [\rho_\infty - \rho_s(0)] \exp \left\{ - \int_0^t \frac{dt'}{\tau(t')} \right\}} \quad (3.15)$$

or

$$\rho_s(0) = \frac{\rho_\infty \rho_s(t) \exp \left\{ - \int_0^t \frac{dt'}{\tau(t')} \right\}}{\rho_\infty - \rho_s(t) + \rho_s(t) \exp \left\{ - \int_0^t \frac{dt'}{\tau(t')} \right\}} \quad (3.16)$$

where $\rho_s(0)$ is the density of sample at the end of the quench. Since $\rho_s(0)$ is a constant, one has that

$$\frac{d\rho_s(0)}{dt} = 0 \quad (3.17)$$

which leads to

$$\tau(t) = \frac{\rho_s(t)[\rho_\infty - \rho_s(t)]}{\rho_\infty \frac{d\rho_s(t)}{dt}} \quad (3.18)$$

where $\frac{d\rho_s(t)}{dt}$ and $\rho_s(t)$ are calculated by Eq.3.10, which associated with a known density ρ_∞ from the calibration. After $\tau(t)$ is determined, $\rho_s(0)$ can be calculated from the experimental data at any time t , by Eq.3.16. These results for $\rho_s(0)$ are shown as the lower lines, Figure 3.3-1. The density $\rho_s(0)$ calculated in this manner agrees well with the value obtained by extrapolating Eq.3.10 to $t=0$.

The time constant $\tau(t)$, the most important factor in the rate equation, must be modeled in some manner in terms of the prior history. In a traditional framework one has factors for the temperature, the pressure (if pressure is a variable) and the non-equilibrium volume. In practice, however, it is difficult to separate these three effects when the cooling rate (or pressure change rate) is very fast. Therefore, a simpler (empirical) approach was taken, in which only one correlating variable ($\Delta\theta_f$) is used. For that purpose the following model is proposed.

$$\tau(t) = \tau_0 \exp\{-\beta (\Delta\theta_f)^n\} \quad (3.19)$$

where

$$\Delta\theta_f = \frac{V_{ng}}{V_0} = 1 - \frac{V + V_0 \alpha_g (T_0 - T)}{V_0} \quad (3.20)$$

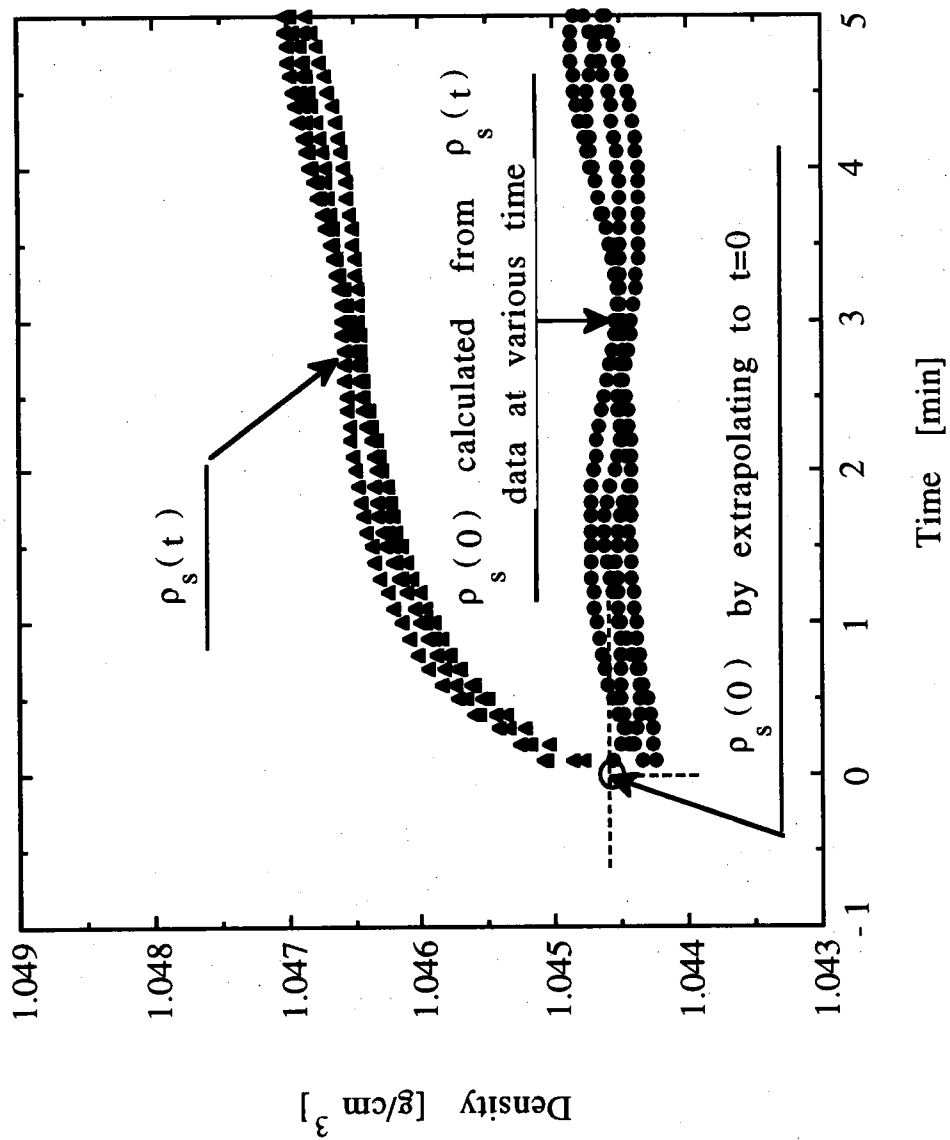


Figure 3.3-1 Density of the quenched samples calculated in various ways

where τ_0 is the time constant at T_0 , β is an adjustable constant, n is a rate-dependent constant, and V_{ng} is a kind of measure of the nonequilibrium free volume, the difference between the two lines shown in Figure 3.3-2. The upper line is the base specific volume adjusted for the glassy change ("occupied volume" change) that one would expect for the temperature there. The middle line is the actual specific volume at that time. The lower line is the equilibrium specific volume. The factor $\Delta\theta_f$ is thus not the free volume as such, but is related to it. V_{ne} is the nonequilibrium free volume. The adjustment of this scheme to different starting temperatures and pressures will be discussed later (Chapter 4). The model has two adjustable constants, β and n , the second of which is taken to be cooling rate dependent. Both β and n were determined by fitting the data of Greiner and Schwarzl[8] (Figure 3.3-3). In present work, also various values of n were assumed so as to fit the calculated density from the DGC at time $t=0$. The assumed empirical index, n , as a function of cooling rate, q , is summarized in Table 3.3-1.

Table 3.3-1 Empirical index (n) as
a function of cooling rate (q)
($-\beta=500$ and $T_0 = 120^\circ\text{C}$)

Range of Cooling Rate (q) [$^\circ\text{C}/\text{sec}$]			Index (n)
∞	--	$< 10^{-5}$	1.00
10^{-5}	--	$< 10^{-2}$	0.95
0.01	--	< 0.1	0.90
0.1	--	< 1	0.86
1	--	< 10	0.83
10	--	< 100	0.80
100	--	∞	0.75

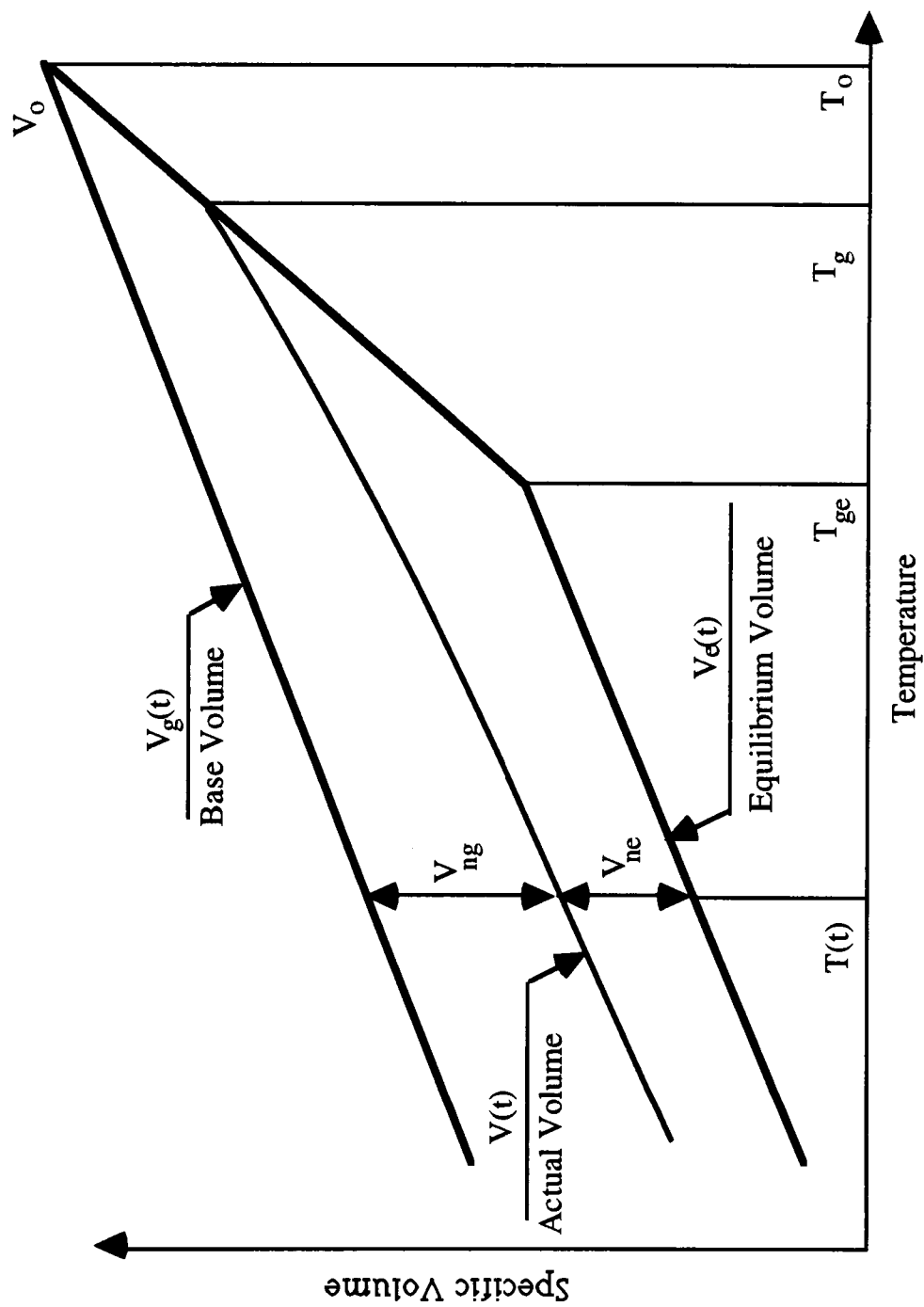


Figure 3.3-2 Qualitative volume-temperature plot of an amorphous polymer

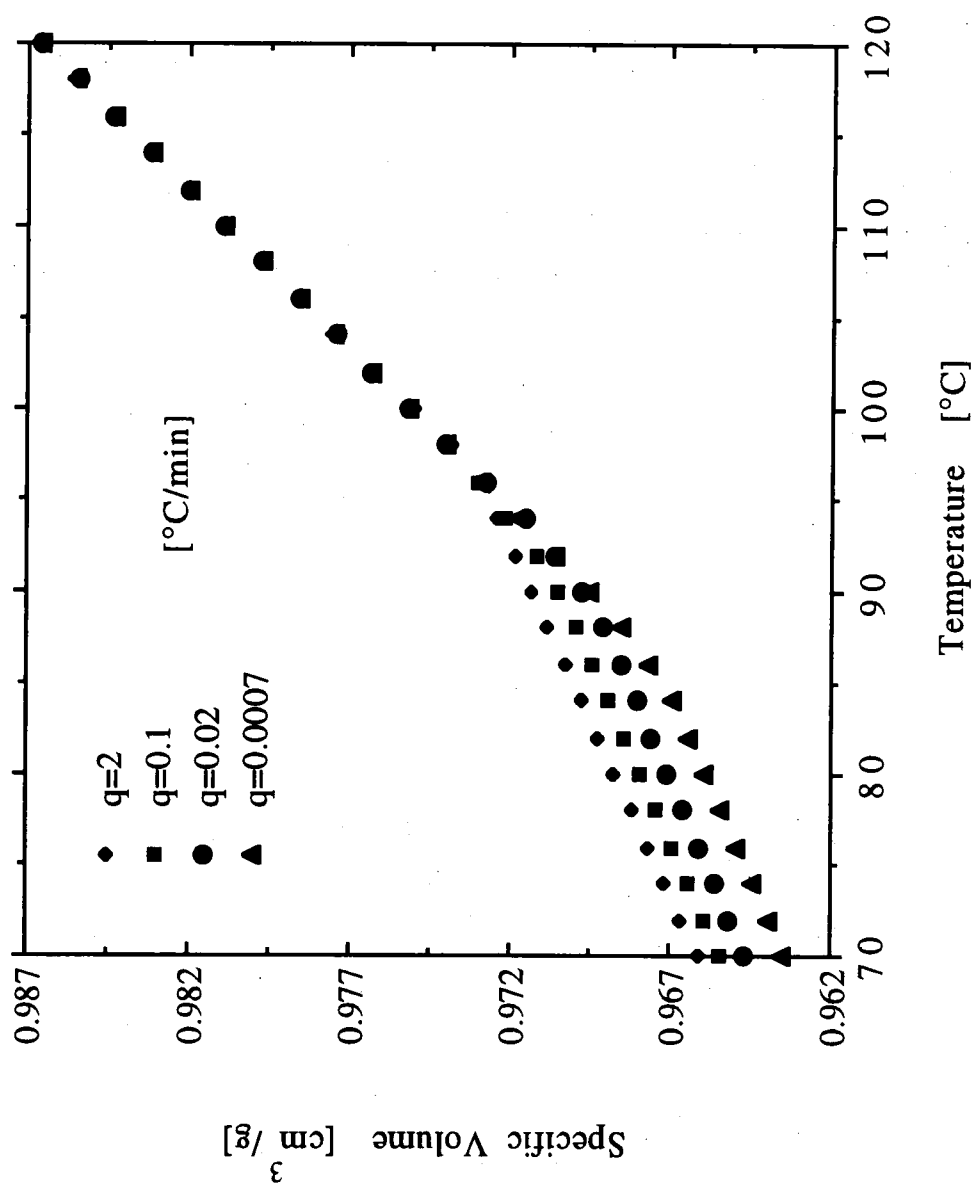


Figure 3.3-3 Specific volume data from Greiner and Schwarzl [8], the cooling rates as those indicated

With these constants available, a prediction of the density changes at various cooling rates can be made. Figure 3.3-4 shows the thermal histories of the samples of the present experiments. Using the cooling rates, Figure 3.3-3, or the thermal histories, Figure 3.3-4, the density changes can be calculated. The results for the two conditions of the present work are given in Figure 3.3-5, in which one notes that the predicted specific volume of the samples are agreed with that available aging data measured by the DGC, that is, data from the aging part of the entire thermal history. Summarized in Figure 3.3-6 are the data of Greiner and Schwarzl with predicted curves, and the predictions from present work. All predictions were calculated by using the rate equation with the time constant model, Eqs. 3.19 and 3.20. This figure, while it includes a number of assumptions, does seem to be a plausible representation of volume changes.

To look at the plausibility (Figures 3.3-5 and 3.3-6), the apparent T_g associated with the various experiments is considered. In the Greiner and Schwarzl case, the apparent T_g is read as the intersection point by extrapolation of the rubbery and glassy portions. These intersection points accompanied a nonequilibrium free volume about $V_{ne} = 0.025$. In the present experiments, the cooling rate is not a constant. But typical values are that several degrees per second for air quench and hundreds of degree per second for water quench. One can determine a temperature—i.e., an apparent T_g —which are obtained from the predicted specific volume curves at which $V_{ne} = 0.025$. The apparent T_g s are summarized in Figure 3.3-7. The agreement between the data of Greiner and Schwarzl and the present data is good.

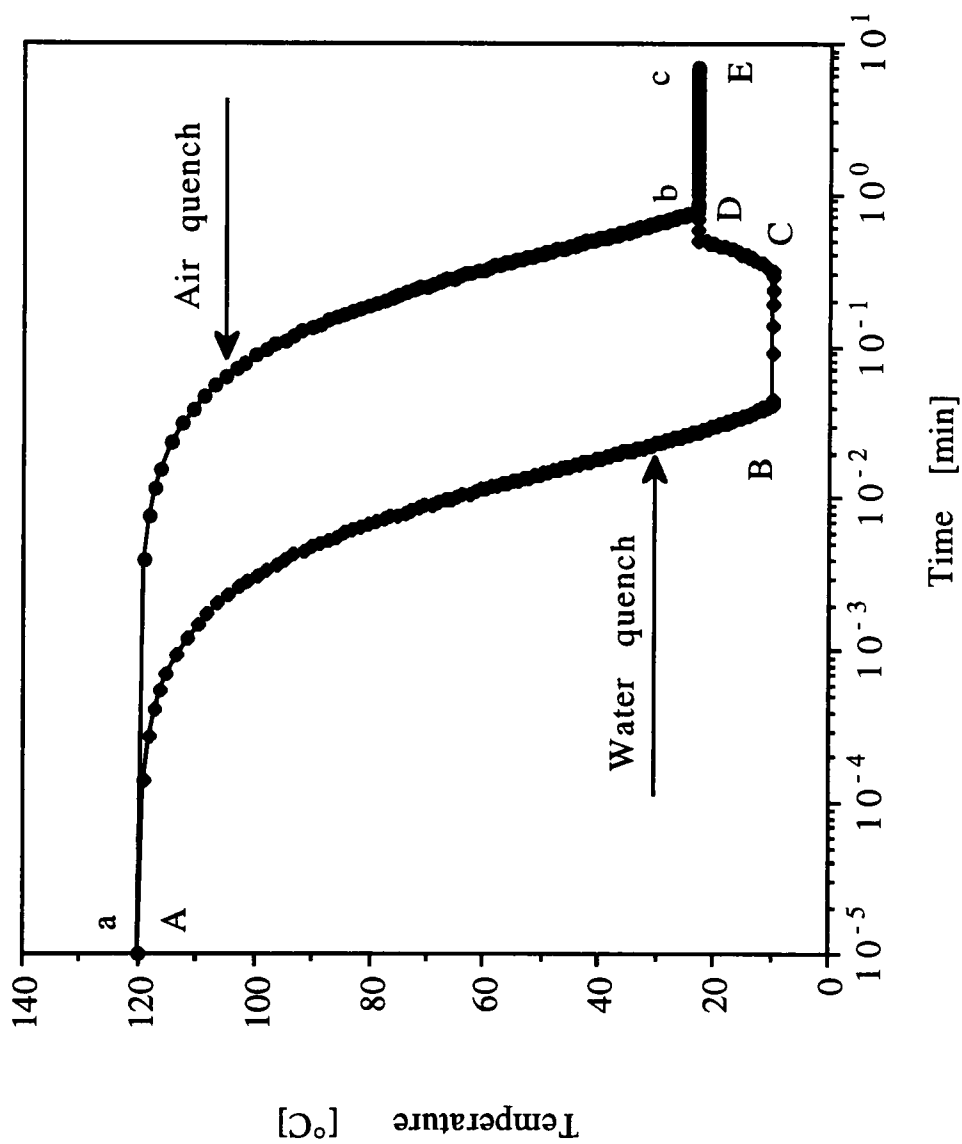


Figure 3.3-4 Thermal histories of the samples during air and water quenches
 ab: air quench, bc: transfer and aging in DGC;
 AB: water quench, BC: in water bath, CDE: transfer and aging in DGC

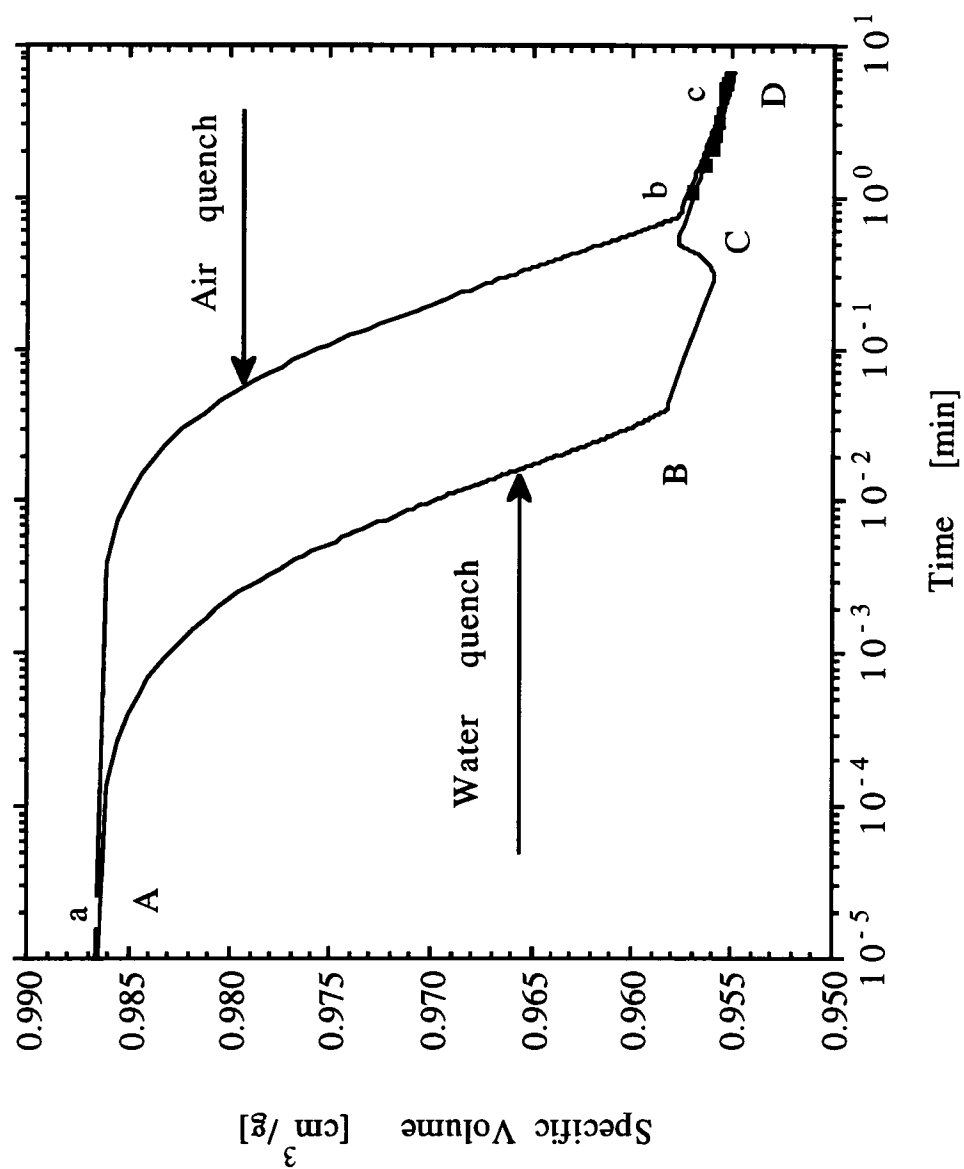


Figure 3.3-5 Specific volume for two quench conditions, labels as those in Figure 3.3-4
 — predictions with present model, ♦ present data from DGC

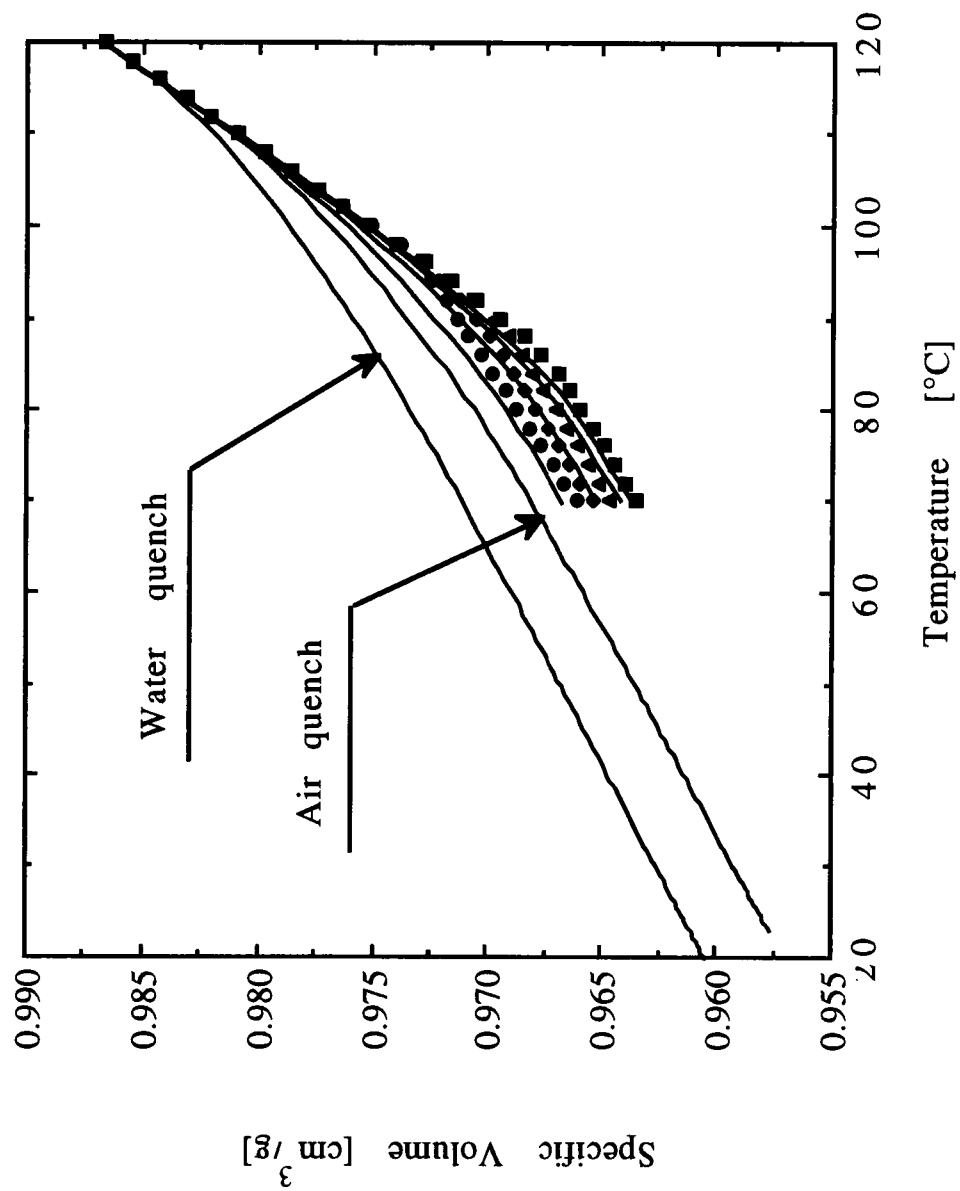


Figure 3.3-6 Fitting of specific volume data with rate equation, the symbols are the same data as in Figure 3.3-3, the curves are predictions based on the rate equation

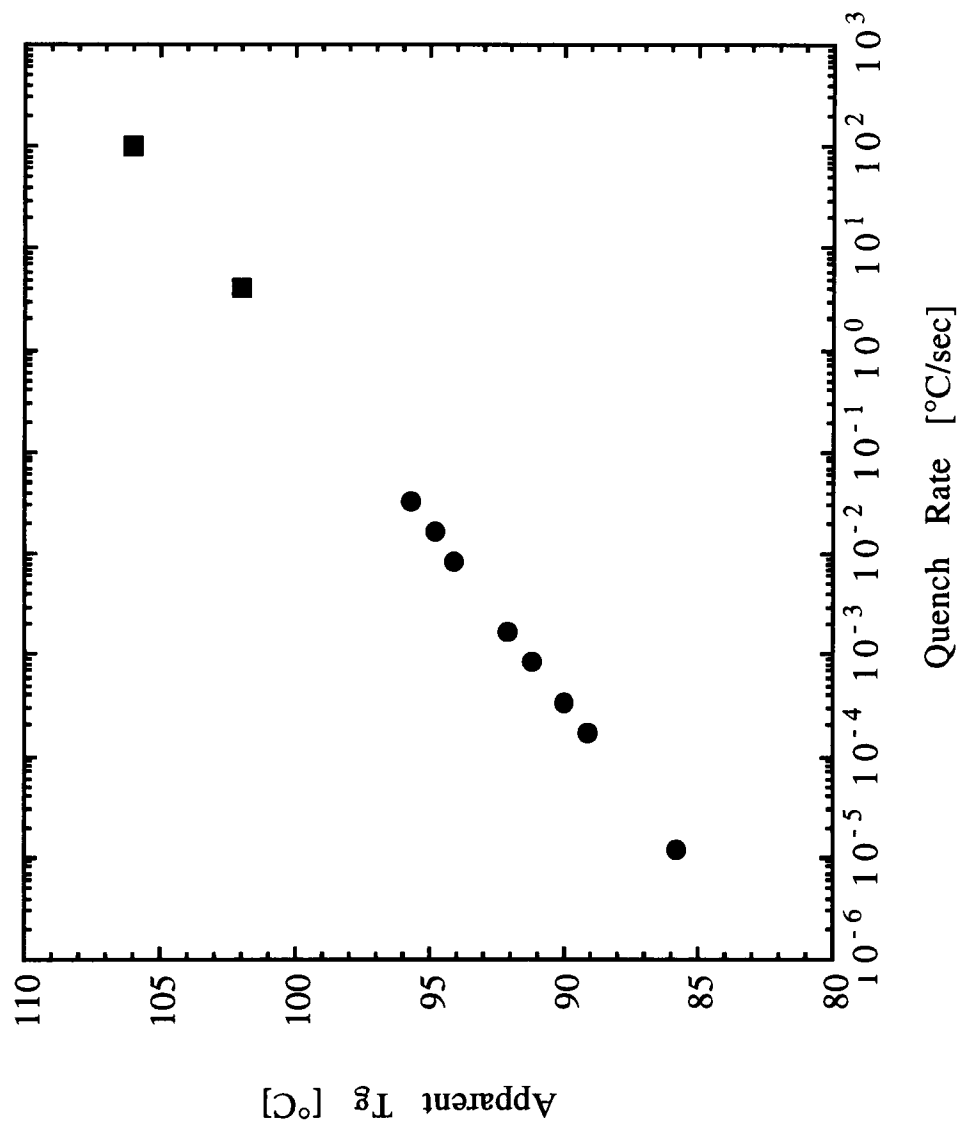


Figure 3.3-7 Apparent T_g as a function of cooling rate,
 • the data of Greiner and Schwarzl[8],
 ■ the data of present experiments

CHAPTER 4

SIMULATION OF VARIOUS STEPS IN INJECTION MOLDING

A complete injection molding process involves several stages, namely, filling, packing, cooling and post-ejection. Computer simulation of injection molding has been attracting research groups for many years. Several commercial software packages for such simulations have already been marketed, such as C-MOLD from AC Technology (Ithaca, New York). But due to a lack of satisfactory theories for describing all of the complicated details, most software packages are not complete, especially as regards effects such as residual stresses. The present work on the simulation of injection molding focused on three steps: packing, cooling and post-ejection, starting with an assumed state at the end of the filling step. This chapter will consist of three sections. In the first part a complete theoretical work for the post-filling steps will be done. In the second part some manipulations of the equations will be presented for purpose of simplification of programming. In the third part there will be the discussion of volume-induced residual stresses. Comparison of simulation with literature data will be made in terms of pressure, specific volume or density, and residual stresses. Also an alternate simulation of the post-ejection step will be presented in this section.

§4.1. Theoretical Work for Various Steps in Injection Molding

The development of residual stresses in polymer parts is an important problem. Such stresses are developed, for example, in injection molding or in other processes in which a large sample is cooled rapidly. The classical residual stress problem has to do with an unconstrained sample, such as when a slab of material is quenched into a water or air bath. This classical problem, however, is not closely related to the problem of injection molding, for which one has a constrained sample inside the mold. In the injection

molding problem, the total volume of the sample is constant—i.e., the volume of the mold—but the specific volume of the material at each point is not constant. It changes in a complicated way as the temperature may change in all steps, and also pressure may change during the filling, cooling and post-ejection steps. This complicated thermal and pressure history produces residual stresses. Also, the residual stresses are strongly dependent on the geometry of the part and on the subsequent aging process. All of the process steps are very complicated because of the inhomogeneity of the temperature, the complicated geometries and the relaxation of the stresses.

In general, a simulation of injection molding should consist of a set of simultaneous equations, that is,

- (1) a continuity equation,
- (2) a force balance equation,
- (3) a torque balance equation,
- (4) an energy equation,
- (5) a PVT equation of state, and
- (6) a constitutive equation for stresses.

In fact, however, the torque balance equation does not appear because it is implied in the symmetry of the stress tensor ($\sigma_{ij} = \sigma_{ji}$). The constitutive equation can be in either integral or differential forms. In general, these equations must be solved simultaneously. But if one deals with very simple cases, they can be simplified and decoupled, as was reviewed in the previous sections (Chapter 2).

In order to simulate the injection molding problem in a tractable way, this work used a simplified geometry—a flat rectangular slab—to which a high temperature and a high hydrostatic pressure were initially applied. These conditions are determined from the filling step. The slab is imagined to consist of many thin layers in the z -direction. At the end of filling it is assumed that the following conditions exist:

- (1) an isotropic pressure profile throughout the whole part, which is the initial packing pressure,

(2) a homogeneous temperature field in the x-y plane, but a temperature gradient in the z-direction due to heat transfer,

(3) a homogeneous density in the x-y plane and a density gradient in the z-direction due to temperature gradients per (2).

Flow-induced orientation effects will not be considered in this work.

With the above conditions and assumptions, the theoretical work will be presented in the following sections.

§4.1.1 Analysis of Heat Transfer in Rectangular Slabs

First, one needs to deal with the energy equation which governs the thermal history of an injection molded slab. The energy equation is, in general, written as[56],

$$\rho C_v \frac{DT}{Dt} = k \frac{\partial^2 T}{\partial x_i^2} + \sigma_{ij} \frac{\partial v_i}{\partial x_j} - T \left(\frac{\partial P}{\partial T} \right) \frac{\partial v_i}{\partial x_i} \quad (4.1)$$

where C_v is the heat capacity per unit volume, k is the thermal conductivity, and ρ is the density. A quantity known as the thermal diffusivity is often used. It is defined as

$$\alpha = \frac{k}{\rho C_v} \quad (4.2)$$

For an essentially solid material (with zero or small velocities), then, the energy equation can be simplified to

$$\begin{aligned} \frac{\partial T}{\partial t} &= \left(\frac{k}{\rho C_v} \right) \frac{\partial^2 T}{\partial x_i^2} \\ &= \alpha \frac{\partial^2 T}{\partial x_i^2} \end{aligned} \quad (4.3)$$

where α is assumed to be a constant. This equation can be solved independently for the temperature profile in a solid slab. The solution of this problem can be found elsewhere[56][84][85].

Two solutions for special cases are restated here. When one deals with an injection molded part during the packing and cooling steps, where the material remains in contact with the wall of the mold, one can use an infinite heat transfer coefficient. In this case the transient temperature is given by

$$\frac{T_w - T(h,t)}{T_w - T_0} = 2 \sum_{m=0}^{\infty} \left\{ \frac{(-1)^m}{(m+\frac{1}{2})\pi} \exp\left[-(m+\frac{1}{2})^2 \pi^2 \frac{\alpha t}{H^2}\right] \cos\left[(m+\frac{1}{2}) \frac{\pi h}{H}\right] \right\} \quad (4.4)$$

where T_w is the surface temperature (a constant temperature), T_0 is the original temperature at $t=0$, H is the half thickness of the slab, h is the distance from the center line to layer i , α is the thermal diffusivity of the solid, and t is the time.

After the molds opened, a finite resistance in the medium surrounding the slab is introduced. A second boundary condition associated with this effect can be rewritten as

$$-k \left(\frac{\partial T}{\partial z} \right) = h_{tc} (T - T_w) \quad h=H \quad (4.5)$$

and

$$-k \left(\frac{\partial T}{\partial z} \right) = -h_{tc} (T - T_w) \quad h=-H \quad (4.6)$$

where h_{tc} is the heat transfer coefficient. The solution is now given as below:

$$\frac{T_w - T(h,t)}{T_w - T_0} = \sum_{m=0}^{\infty} \left\{ \frac{2 \sin(\lambda_m)}{\lambda_m + \sin(\lambda_m) \cos(\lambda_m)} \exp\left[-(\lambda_m)^2 \frac{\alpha t}{H^2}\right] \cos\left[\frac{\lambda_m h}{H}\right] \right\} \quad (4.7)$$

where λ_m are the roots of Equation 4.8, and N_{Bi} is the Biot number defined by Equation 4.9.

$$\lambda_m \sin(\lambda_m) = N_{Bi} \cos(\lambda_m) \quad (4.8)$$

$$N_{Bi} = \frac{h_{tc} h}{k} \quad (4.9)$$

Equation 4.7 converges slowly. To avoid this problem, there are two other alternate forms of Equation 4.7 [38][84], namely,

$$\frac{T_w - T(h,t)}{T_w - T_0} = \sum_{m=0}^{\infty} \left\{ \frac{2 N_{Bi}}{(\lambda_m)^2 + \cos(\lambda_m) (N_{Bi} (N_{Bi} + 1))} \exp\left[-(\lambda_m)^2 \frac{\alpha t}{H^2}\right] \cos\left[\frac{\lambda_m h}{H}\right] \right\} \quad (4.10)$$

and

$$\begin{aligned} \frac{T_w - T(h,t)}{T_w - T_0} = & 1 - \operatorname{erfc}\left\{\frac{H-h}{2\sqrt{\alpha t}}\right\} - \operatorname{erfc}\left\{\frac{H+h}{2\sqrt{\alpha t}}\right\} \\ & + \exp\left[\frac{h_{tc}}{k}(H-h) + \left(\frac{h_{tc}}{k}\right)^2 (\alpha t)\right] \\ & \operatorname{erfc}\left\{\frac{h_{tc}}{k}\sqrt{\alpha t} + \frac{H-h}{2\sqrt{\alpha t}}\right\} \\ & + \exp\left[\frac{h_{tc}}{k}(H+h) + \left(\frac{h_{tc}}{k}\right)^2 (\alpha t)\right] \\ & \operatorname{erfc}\left\{\frac{h_{tc}}{k}\sqrt{\alpha t} + \frac{H+h}{2\sqrt{\alpha t}}\right\} \end{aligned} \quad (4.11)$$

where $\text{erf}(x)$ is the error function and $\text{erfc}(x) = 1 - \text{erf}(x)$ is the complementary error function.

The rate of the temperature change can be obtained from these equations by differentiating either analytically (Eq. 4.4) or numerically (Eqs. 4.10 and 4.11). Equations 4.4 and 4.11 will be used in the simulation programming later.

§4.1.2 Analysis of Various Steps in Injection Molding

With the known thermal history from the prior section, an analysis of packing, cooling and post-ejection steps is presented below.

The formulation for residual stresses produced in a constrained sample (inside the mold) consists of a set of equations as mentioned at the beginning of this chapter, except that the torque balance equation and the energy equation have been dealt with separately. The remaining equations are discussed below.

1. A generalized PVT equation:

$$\frac{D(\theta + \phi_f)}{Dt} = -\frac{\Delta\theta}{\tau(t)} \quad (4.12)$$

or,

$$\begin{aligned} \frac{dV}{dt} &= -\frac{V_{ne}(T,P)}{\tau(t)} + V_s \alpha_a \frac{dT}{dt} - V_s \kappa_a \frac{dP}{dt} \\ &= -\frac{V - V_e}{\tau(t)} + V_s \alpha_a \frac{dT}{dt} - V_s \kappa_a \frac{dP}{dt} \end{aligned} \quad (4.13)$$

where the time constant is

$$\begin{aligned} \tau(t) &= \tau_0 a_s a_f \\ &= \tau_0 \exp\{-\beta (\Delta\theta_s)\} \exp\{-\beta (\Delta\theta_f)^n\} \end{aligned} \quad (4.14)$$

where

$$\Delta\theta_f = 1 - \frac{V + V_s \alpha_g (T_s - T) - V_s \kappa_g [P_s - P(t)]}{V_s} \quad (4.15)$$

$$\Delta\theta_s = 1 - \frac{V_s + V_0 \alpha_g (T_0 - T_s) - V_0 \kappa_g (P_0 - P_s)}{V_0} \quad (4.16)$$

$$V_e(T, P) = V_0 [1 - \alpha_r (T_0 - T(t)) + \kappa_r (P_0 - P(t))] \quad T > T_{ge} \quad (4.17)$$

$$V_e(T, P) = V_0 [1 - \alpha_r (T_0 - T_{ge}) - \alpha_g (T_{ge} - T(t)) + \Delta\kappa (P_0 - P(t))] \quad T < T_{ge} \quad (4.18)$$

where $V_e(T, P)$ is the equilibrium specific volume at the conditions of the temperature T and the pressure P ; τ_0 is the reference time constant at the reference condition T_0, P_0 ; a_f is the shift factor of the time constant for the nonequilibrium volume; $\Delta\theta_f$ is the correlating variable related to the nonequilibrium volume; β is an adjustable constant for time constant, and n is the rate-dependent constant; α_r and α_g are the thermal coefficients of volumetric expansion for the rubbery and glassy states, respectively; κ_r and κ_g are the pressure coefficients of volumetric expansion for rubbery and glassy states, respectively; α_a is an average thermal coefficient of volumetric expansion, and κ_a is an average pressure coefficient of volumetric expansion. V_0 means $V_e(T_0, P_0)$, the reference specific volume at T_0, P_0 ; V_s means $V_e(T_s, P_s)$, the starting specific volume (initial specific volume) at T_s, P_s ; $\Delta\theta_s$ is the initial value of $\Delta\theta_f$ for the different starting temperature and pressure; and a_s is the initial value of a_f . It is assumed that equilibrium glass transition temperature T_{ge} is pressure-dependent only[79]. The volume changes are linearized around the V_0 and V_s , respectively.

Figure 4.1-1 is a PVT plot of an amorphous polymer which shows that the time constant is shifted to a different starting temperature and pressure. In this plot two sets of solid lines present two constant pressure values, P_0 and P_s .

2. A continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho v_i)}{\partial x_i} = 0 \quad (4.19)$$

Since the present work on injection molding deals with only the post-filling steps, $v_x = v_y = 0$, only the velocity v_z plays a role in Eq. 4.19. The final form of the continuity equation is thus

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho v_z)}{\partial z} = 0 \quad (4.20)$$

3. A generalized anisotropic stress equation:

$$\sigma'_{ij} + \tau_g(T, t) \frac{D \sigma'_{ij}}{Dt} = G(t) \tau_g(T, t) d_{ij}^* \quad (4.21)$$

where

$$\sigma_{ij} = -P \delta_{ij} + \sigma'_{ij} \quad (4.22)$$

$$d_{ij}^* = \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} - \frac{2}{3} \frac{\partial v_k}{\partial x_k} \delta_{ij} \quad (4.23)$$

$$\frac{D \sigma'_{ij}}{Dt} = \frac{D \sigma'_{ij}}{Dt} - \left(\frac{\partial v_i}{\partial x_k} \sigma'_{kj} + \frac{\partial v_j}{\partial x_k} \sigma'_{ik} \right) \quad (4.24)$$

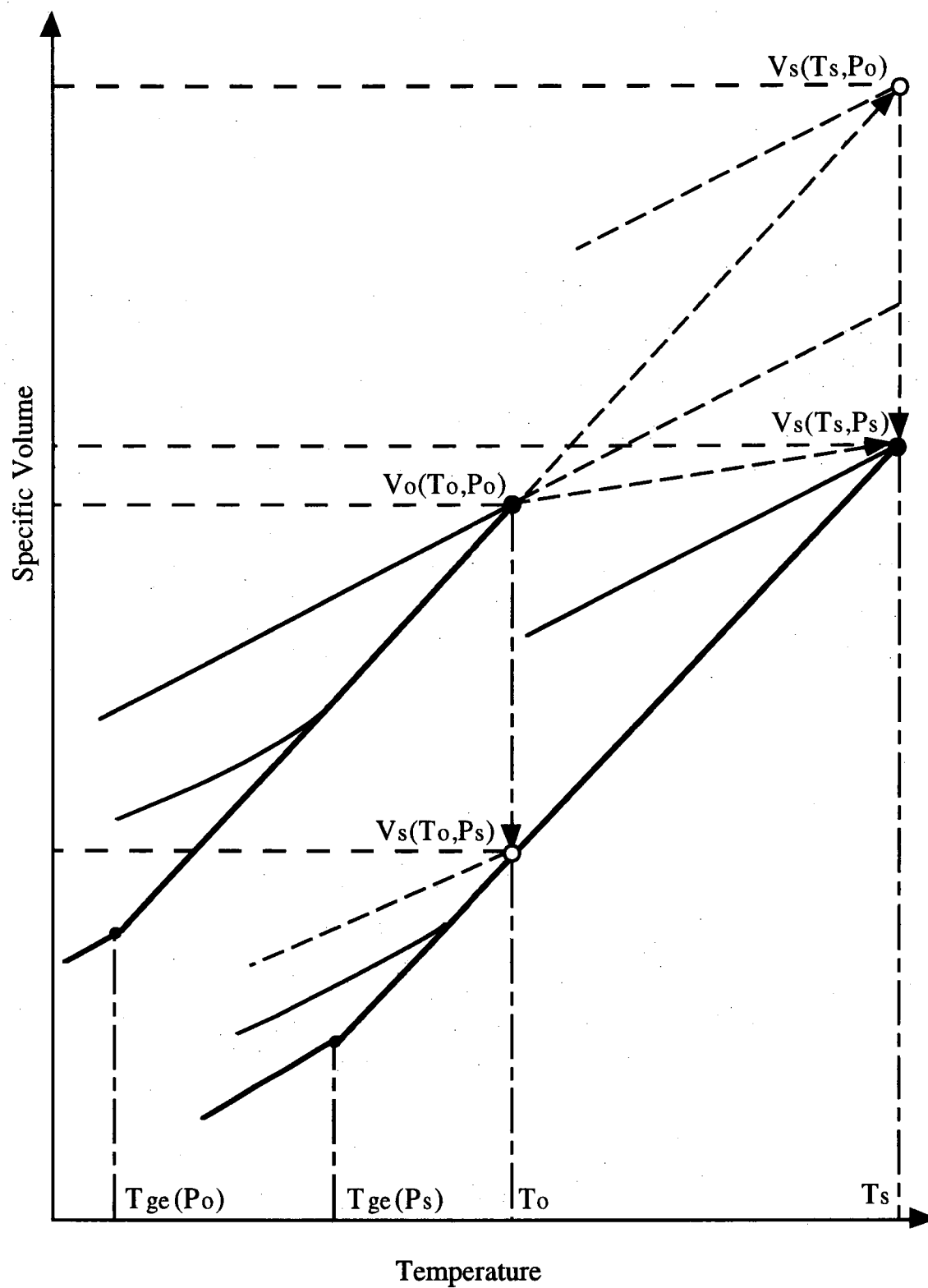


Figure 4.1-1 Qualitative PVT plot of an amorphous polymer

$$\frac{D\sigma'_{ij}}{Dt} = \frac{\partial \sigma'_{ij}}{\partial t} + v_k \frac{\partial \sigma'_{ij}}{\partial x_k} \quad (4.25)$$

$$\tau_G(t) = \tau_{G0} a_G(T) \quad (4.26)$$

where τ_{G0} is the time constant for stress changes at a reference temperature, T_r ; $a_G(T)$ is a shift factor which is temperature (and thus time) dependent; $G(t)$ is the elastic modulus, which is assumed to be temperature-dependent only[54][62] as shown in Figure 4.1-2;

σ'_{ij} is the extra stress, $\frac{\delta \sigma'_{ij}}{\delta t}$ is a contravariant derivative, (the so-called "upper" convected derivative), and d_{ij}^* is a normalized deformation rate tensor. Both $G(t)$ and $\tau_G(t)$ are functions of temperature (and thus of time). The key idea of the present framework, initially proposed by Ko and Bogue[4], is to introduce an isotropic pressure P . The total stresses σ_{ij} are composed of two components, isotropic stress $-P$ and anisotropic stress σ'_{ij} . Recalling that $v_x = v_y = 0$ and v_z is independent of x and y , one has that $\sigma'_{xy} = \sigma'_{yz} = \sigma'_{zx} = 0$, and the set of generalized anisotropic stresses reduces to the following three equations:

$$\sigma'_{xx} + \tau_G(T, t) \frac{\delta \sigma'_{xx}}{\delta t} = G(t) \tau_G(T, t) d_{xx}^* \quad (4.27)$$

$$\sigma'_{yy} + \tau_G(T, t) \frac{\delta \sigma'_{yy}}{\delta t} = G(t) \tau_G(T, t) d_{yy}^* \quad (4.28)$$

$$\sigma'_{zz} + \tau_G(T, t) \frac{\delta \sigma'_{zz}}{\delta t} = G(t) \tau_G(T, t) d_{zz}^* \quad (4.29)$$

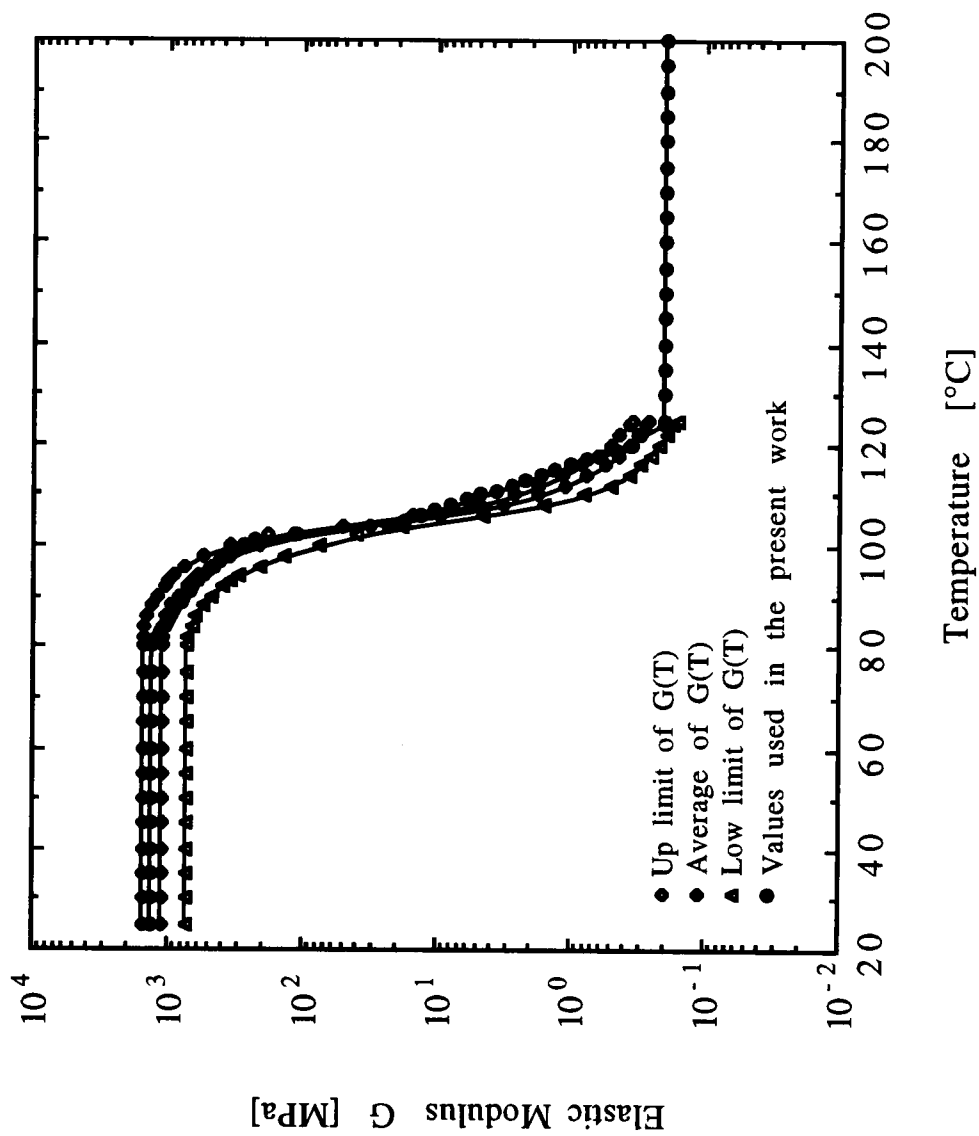


Figure 4.1-2 Elastic modulus $G(T)$ as a function of temperature[54][62]

4. A force balance equation:

For an individual layer i in z -direction, one has a force balance equation as below:

$$m_i \frac{dv(i,t)}{dt} = \Delta\sigma_{zz}(i,t) + m_i g_z \quad (4.30)$$

where σ_{zz} is defined by Eq.4.22, m_i is the mass, $v(i,t)$ is the velocity, and $\Delta\sigma_{zz}(i,t)$ is the difference of the stresses between two surfaces of the layer in the z -direction (where $z=0$ is the center of the sample). In present study, the inertial and gravitational terms are negligible. Thus the force balance equation reduces to the simple form:

$$\begin{aligned} \Delta\sigma_{zz}(i,t) &= \Delta\{-P\delta_{zz} + \sigma'_{zz}\} \\ &= -P(i+1,t) + \sigma'_{zz}(i+1,t) + P(i,t) - \sigma'_{zz}(i,t) \\ &= 0 \end{aligned} \quad (4.31)$$

The coupled equations for injection molding for the post-filling steps are summarized in Table 4.1-1.

§4.1.3 Analysis of Constraint Conditions for Simulation

To solve above differential equations, one needs associated boundary conditions. The constraint conditions are different for the three steps of the post-filling. The analysis of them is given below.

1. Packing step:

The first constraint condition for the packing step is related to the fact that the total volume of the cavity, V_{cavity} , is constant.

Table 4.1-1

Summary of coupled equations for the post-filling steps in injection molding

Equation	Notes
$\Delta\{\sigma_{zz}(i,t)\} = \Delta\{-P(i,t) + \sigma'_{zz}(i,t)\} = 0$	<u>Force Equation</u>
$\sigma'_{xx} + \tau_g(T,t) \frac{\partial \sigma'_{xx}}{\partial t} = G(t) \tau_g(T,t) d_{xx}^*$	<u>Constitutive Equation</u> where $\sigma'_{xy} = \sigma'_{yz} = \sigma'_{xz} = 0$
$\sigma'_{yy} + \tau_g(T,t) \frac{\partial \sigma'_{yy}}{\partial t} = G(t) \tau_g(T,t) d_{yy}^*$	
$\sigma'_{zz} + \tau_g(T,t) \frac{\partial \sigma'_{zz}}{\partial t} = G(t) \tau_g(T,t) d_{zz}^*$	
$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho v_z)}{\partial z} = 0$	<u>Continuity Equation</u> where $v_x = v_y = 0$
$\frac{dV}{dt} = -\frac{V - V_e}{\tau(t)} + V_s \alpha_{ad} \frac{dT}{dt} - V_s \kappa_{ad} \frac{dP}{dt}$	<u>PVT-time Equation</u>

Table 4.1-1 (continued)

Equation	Notes
$\frac{T_w - T(h, t)}{T_w - T_0} = 2 \sum_{m=0}^{\infty} \left\{ \frac{(-1)^m}{(m + \frac{1}{2})\pi} \exp \left[-\left(m + \frac{1}{2}\right)^2 \pi^2 \frac{2\alpha t}{H^2} \right] \cos \left[\left(m + \frac{1}{2}\right) \frac{\pi h}{H} \right] \right\}$	<u>Heat Transfer Equation</u> with infinite heat transfer coefficient for packing and cooling steps.
$\begin{aligned} \frac{T_w - T(h, t)}{T_w - T_0} = & 1 - \operatorname{erfc} \left\{ \frac{H-h}{2\sqrt{\alpha t}} \right\} - \operatorname{erfc} \left\{ \frac{H+h}{2\sqrt{\alpha t}} \right\} \\ & + \exp \left[\frac{h_{tc}}{k} (H-h) + \left(\frac{h_{tc}}{k} \right)^2 (\alpha t) \right] \operatorname{erfc} \left\{ \frac{h_{tc}}{k} \sqrt{\alpha t} + \frac{H-h}{2\sqrt{\alpha t}} \right\} \\ & + \exp \left[\frac{h_{tc}}{k} (H+h) + \left(\frac{h_{tc}}{k} \right)^2 (\alpha t) \right] \operatorname{erfc} \left\{ \frac{h_{tc}}{k} \sqrt{\alpha t} + \frac{H+h}{2\sqrt{\alpha t}} \right\} \end{aligned}$	<u>Heat Transfer Equation</u> with finite heat transfer coefficient for post-injection step.

$$\sum_{i=1}^N V(i,t) = V_{\text{cavity}} \quad (4.32)$$

where $V(i,t)$ refers to the specific volume of the imagined layer i , and N is the total number of the imagined layers. $V(i,t)$ is position and time dependent. This equation has to be satisfied during packing.

The second constraint condition is related to the fact that the packing pressure is a known processing condition, which is decided at the end of the filling. The pressure $P_{\text{pack}}(t)$ is a known prescribed function of time and is the same in all layers. To achieve this condition one must imagine that a small amount of mass is added to each layer. This amount of added (or readjusted) mass is not expectantly calculated since the constraints are ones of known pressure and temperature, but not density, which is a dependent variable. Since the layers are assumed to be homogenous in the x-y plane, the mass must be imagined to be distributed uniformly throughout each layer. More mass must be added to the layers that have a larger temperature decrease. These layers are intermediate between the wall and the centerline, because the layers very near the wall have already cooled and the layers near the centerline are still near the original melt temperature. This must be what happens physically in an actual packing process, although the flow patterns are very complicated, involving movement from the center to the outside. In other words, the present simulation appears to be a reasonable approximation to the pressure/density history in an overall sense, though not in detail. Therefore, the second constraint condition for packing step is,

$$-\sigma_{zz}(i, t) = P_{\text{pack}}(t) \quad (4.33)$$

2. Cooling step:

During the cooling step, the total stress is changing, i.e., packing is no longer an independent variable. The first constraint condition is that the total volume of the cavity is constant. Equation 4.32 is still valid here. The total mass of the molded part now becomes constant, the same as that at the end of the packing. Letting M be this constant mass, one then has the second constraint condition

$$\sum_{i=1}^N m_i = M \quad (4.34)$$

where m_i is the mass of layer i , and N is the total number of the imagined layers.

3. Post-ejection step:

The post-ejection step is the time period after the mold is opened (after the part is ejected from the mold). To deal with an ejected part, one has to note two important facts. The first fact is that the ejected part is no longer in contact with the wall of the mold. The part is now exposed to a different environmental thermal condition, requiring a new treatment of the energy equation. This has been dealt with in Section §4.1.1 in terms of a finite heat transfer resistance. The second fact is that the sample is no longer constrained after ejected. Its dimensions are changing in all directions. However, each layer in the z -direction changes its thickness differently, giving a total thickness $L_z(t)$. The long dimensions of these layers are presumed to be the same in all layers in the x -direction and y -direction (that is, $L_x(i,t)=L_x(t)$, and $L_y(i,t)=L_y(t)$ for all layers).

After the mold is opened, the total mass of the part still remains constant, so that Equation 4.34 continues to hold. But the total volume of the part varies—i.e., Equation 4.32 no longer holds.

Table 4.1-2
Summary of constraints used in the simulation
of the post-filling steps in injection molding

Step	Constraint	Equation	Note
Packing	• constant total volume	$\sum_{i=1}^N V_i = V_{\text{cavity}}$	The total volume is that of the mold. A small amount of mass is imagined to be added to the cavity to obtain
	• prescribed packing pressure	$-\sigma_{zz}(i, t) = P_{\text{pack}}(t)$	the desired packing pressure.
Cooling	• constant total volume	$\sum_{i=1}^N V_i = V_{\text{cavity}}$	The total volume is that of the mold. The total mass of the molded part remains constant, the same as that at the end of packing.
	• constant total mass	$\sum_{i=1}^N m_i = M$	
Post-ejection	• constant total mass	$\sum_{i=1}^N m_i = M$	The total mass remains constant, the same as that at the end of packing, but the total volume varies. The applied pressure throughout the part is atmospheric.
	• zero applied pressure	$-\sigma_{zz}(i, t) = 0$	

During this step, one knows that the applied pressure throughout the part is atmospheric. This constraint condition can be written as

$$-\sigma_{zz}(i, t) = 0 \quad (4.35)$$

The constraint conditions used in the simulation of the three steps of injection molding are summarized in Table 4.1-2. These constraint equations and the coupled equations summarized in Table 4.1-1 give the complete formulation. They must be solved simultaneously.

§4.2 Formulation for Computer Programming

To execute the simulation on the computer, one may rearrange some of the equations to ease the programming and to run it efficiently. These details are described below.

1. The continuity equation:

The continuity equation, Eq. 4.20, can be written as

$$\frac{\partial v_z}{\partial z} = -\frac{1}{\rho} \left[\frac{\partial \rho}{\partial t} + v_z \frac{\partial \rho}{\partial z} \right] \quad (4.36)$$

In term of specific volume $V(i,t)$, one has

$$-\frac{1}{\rho} \frac{\partial \rho}{\partial t} = \frac{1}{V} \frac{\partial V}{\partial t} \quad (4.37)$$

and

$$-\frac{v_z}{\rho} \frac{\partial \rho}{\partial z} = \frac{v_z}{V} \frac{\partial V}{\partial z} \quad (4.38)$$

so, Eq. 4.36 can be rearranged and the continuity equation reads

$$\frac{\partial v_z}{\partial z} = \frac{1}{V} \frac{\partial V}{\partial t} + \frac{v_z}{V} \frac{\partial V}{\partial z} \quad (4.39)$$

If the partial derivatives are replaced by the first-order finite difference approximation, one has

$$\frac{\Delta v_z}{\Delta z} = \frac{1}{V(i,t)} \frac{\Delta V}{\Delta t} + \frac{v_z(i,t)}{V(i,t)} \frac{\Delta V}{\Delta z} \quad (4.40)$$

that is,

$$\begin{aligned} \frac{\Delta v_z}{\Delta z} &= \frac{v_z(i,t) - v_z(i-1,t)}{\Delta z} \\ &= \frac{V(i,t) - V(i,t-1)}{V(i,t)\Delta t} + v_z(i,t) \frac{V(i,t) - V(i-1,t)}{V(i,t)\Delta z} \end{aligned} \quad (4.41)$$

If Δz is replaced by $\Delta h \equiv (h(i+1) - h(i))$, finally, one has,

$$v_z(i,t) = v_z(i-1,t) \frac{V(i,t)}{V(i-1,t)} + \Delta h \frac{V(i,t) - V(i,t-1)}{V(i-1,t)\Delta t} \quad (4.42)$$

Equations 4.41 and 4.42 will be used in the rearrangement of the stress equation, as shown next.

2. The stress equation:

The normalized components of the deformation rate tensor are

$$d_{xx}^* = \frac{\partial v_x}{\partial x} + \frac{\partial v_x}{\partial x} - \frac{2}{3} \frac{\partial v_z}{\partial z} = -\frac{2}{3} \frac{\partial v_z}{\partial z} \quad (4.43)$$

$$d_{yy}^* = \frac{\partial v_y}{\partial y} + \frac{\partial v_y}{\partial y} - \frac{2}{3} \frac{\partial v_z}{\partial z} = -\frac{2}{3} \frac{\partial v_z}{\partial z} \quad (4.44)$$

$$d_{zz}^* = \frac{\partial v_z}{\partial z} + \frac{\partial v_z}{\partial z} - \frac{2}{3} \frac{\partial v_z}{\partial z} = +\frac{4}{3} \frac{\partial v_z}{\partial z} \quad (4.45)$$

The analysis in terms of contravariant convected derivative gives

$$\frac{\delta \sigma'_{xx}}{\delta t} = \frac{\partial \sigma'_{xx}}{\partial t} + v_z \frac{\partial \sigma'_{xx}}{\partial z} \quad (4.46)$$

$$\frac{\delta \sigma'_{yy}}{\delta t} = \frac{\partial \sigma'_{yy}}{\partial t} + v_z \frac{\partial \sigma'_{yy}}{\partial z} \quad (4.47)$$

$$\frac{\delta \sigma'_{zz}}{\delta t} = \frac{\partial \sigma'_{zz}}{\partial t} + v_z \frac{\partial \sigma'_{zz}}{\partial z} - 2 \frac{\partial v_z}{\partial z} \sigma'_{zz} \quad (4.48)$$

Finally, the extra stress equations become

$$\begin{aligned} \sigma'_{xx} + \tau_G(t) \left[\frac{\partial \sigma'_{xx}}{\partial t} + v_z \frac{\partial \sigma'_{xx}}{\partial z} \right] \\ = G(t) \tau_G(t) \left[-\frac{2}{3} \frac{\partial v_z}{\partial z} \right] \end{aligned} \quad (4.49)$$

$$\begin{aligned} \sigma'_{yy} + \tau_G(t) \left[\frac{\partial \sigma'_{yy}}{\partial t} + v_z \frac{\partial \sigma'_{yy}}{\partial z} \right] \\ = G(t) \tau_G(t) \left[-\frac{2}{3} \frac{\partial v_z}{\partial z} \right] \end{aligned} \quad (4.50)$$

$$\begin{aligned} \sigma'_{zz} + \tau_G(t) \left[\frac{\partial \sigma'_{zz}}{\partial t} + v_z \frac{\partial \sigma'_{zz}}{\partial z} - 2 \frac{\partial v_z}{\partial z} \sigma'_{zz} \right] \\ = G(t) \tau_G(t) \left[+ \frac{4}{3} \frac{\partial v_z}{\partial z} \right] \end{aligned} \quad (4.51)$$

Solving these equations for the time derivatives gives

$$\frac{\partial \sigma'_{xx}}{\partial t} = -\frac{2}{3} G(t) \frac{\partial v_z}{\partial z} - v_z \frac{\partial \sigma'_{xx}}{\partial z} - \frac{\sigma'_{xx}}{\tau_G(t)} \quad (4.52)$$

$$\frac{\partial \sigma'_{yy}}{\partial t} = -\frac{2}{3} G(t) \frac{\partial v_z}{\partial z} - v_z \frac{\partial \sigma'_{yy}}{\partial z} - \frac{\sigma'_{yy}}{\tau_G(t)} \quad (4.53)$$

$$\frac{\partial \sigma'_{zz}}{\partial t} = \left[\frac{4}{3} G(t) + 2\sigma'_{zz} \right] \frac{\partial v_z}{\partial z} - v_z \frac{\partial \sigma'_{zz}}{\partial z} - \frac{\sigma'_{zz}}{\tau_G(t)} \quad (4.54)$$

The partial derivatives in space are replaced by a finite difference approximation, giving

$$\frac{\partial \sigma'_{xx}}{\partial t} = \frac{\partial \sigma'_{yy}}{\partial t} \approx -\frac{2}{3} G(t) \frac{\Delta v_z}{\Delta z} - v_z \frac{\Delta \sigma'_{xx}}{\Delta z} - \frac{\sigma'_{xx}}{\tau_G(t)} \quad (4.55)$$

$$\frac{\partial \sigma'_{zz}}{\partial t} \approx \left[\frac{4}{3} G(t) + 2\sigma'_{zz} \right] \frac{\Delta v_z}{\Delta z} - v_z \frac{\Delta \sigma'_{zz}}{\Delta z} - \frac{\sigma'_{zz}}{\tau_G(t)} \quad (4.56)$$

Substituting Eqs 4.41 and 4.42 into Eqs. 4.55 and 4.56 yields a set of equations for calculating the extra stresses. The PVT-time equation, Eq. 4.13, can be rewritten as

$$\frac{dP}{dt} = \frac{1}{V_s \kappa_a} \left\{ -\frac{V - V_e}{\tau(t)} + V_s \alpha_a \frac{dT}{dt} - \frac{dV}{dt} \right\} \quad (4.57)$$

It needs to be noted that the only purpose of this kind of

rearrangement is to reduce the programming and computing time. Nothing has been changed about the framework. The equations must be solved simultaneously, as stated before.

Although the equations have been rearranged, special calculation techniques are needed to solve them on the computer, because this is a multiple variable problem subject to some constraint conditions[83]. A combination of optimization techniques using linear and multimodal search procedures is employed. The objective of the optimization is that the calculated total stress satisfies the constraint conditions. The programming charts are provided in Figures 4.2-1, 4.2-2 and 4.2-3. The index i identifies each layer, j is the time index, and k is the iteration index. The computer programs are presented in the appendices. The optimum procedures for the objective are briefly summarized as follows:

- (1) Give initial values for all variables, parameters and constants for all layers; start an iteration (k);

- (2) Solve energy equation independently for temperature profiles for all layers at time $t(j)$;

- (3) Initiate a set of small increments in specific volume for layer (i) at time $t(j)$, which is evaluating by a pre-set criterion to satisfy the constraint conditions;

- (4) Solve for pressures and stresses for all layers with a fourth-order Runge-Kutta method;

- (5) Check the objective; if the objective is minimum, shift to step (6); if not, optimize the set of the increments with satisfying the constraint conditions and repeat the procedures from step (4);

- (6) Adjust some variables, parameters and constants to new values based on the results of steps (4) and (5); if all layers have been optimized, shift to step (8) to do another evaluation; if not, continue next step for layer ($i+1$);

- (7) Initiate a new set of small increments in specific volume for layer ($i+1$) at time $t(j)$ with satisfying the constraint conditions; repeat the optimization procedures from step (4);

- (8) Evaluate the objective by a pre-selected criterion; if the

evaluation is pass, output the results of the optimization and shift to step (10); if not, continue next step for iteration (k+1);

(9) Initiate a new set of small increments in specific volume for layer (i) at time t(j) with satisfying the constraint conditions; launch a new iteration (k+1) by repeating the optimization procedures from step (4);

(10) Inspect if all time steps have been simulated. If not, continue next time step (j+1) from step (2); If yes, finish the simulation.

Several search methods have been combined and employed for the optimization. In practice, when a one-dimensional search was conducted, the Golden Section method was applied; When a multivariable problem was related, a multimodal search procedure was employed. The Golden Section is based on the constant 0.618. This section method locates a search point sequentially in 0.618 of the remaining uncertainty. The multimodal search procedure involves repeated sectioning and using different incremental step sizes. More details about the optimization and the multimodal search procedures can be found elsewhere[83][91][92][93].

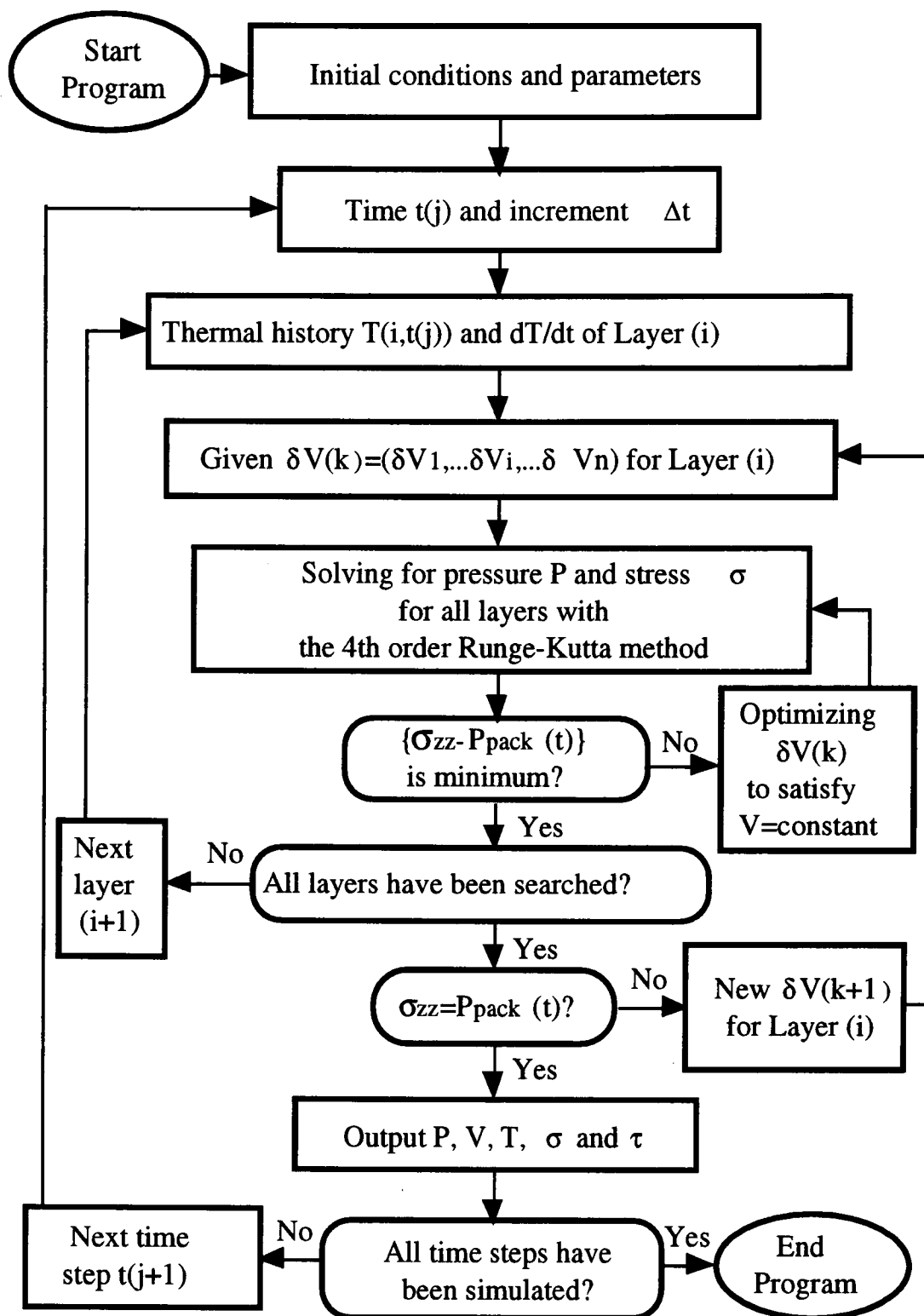


Figure 4.2-1. Programming chart-I for the packing step

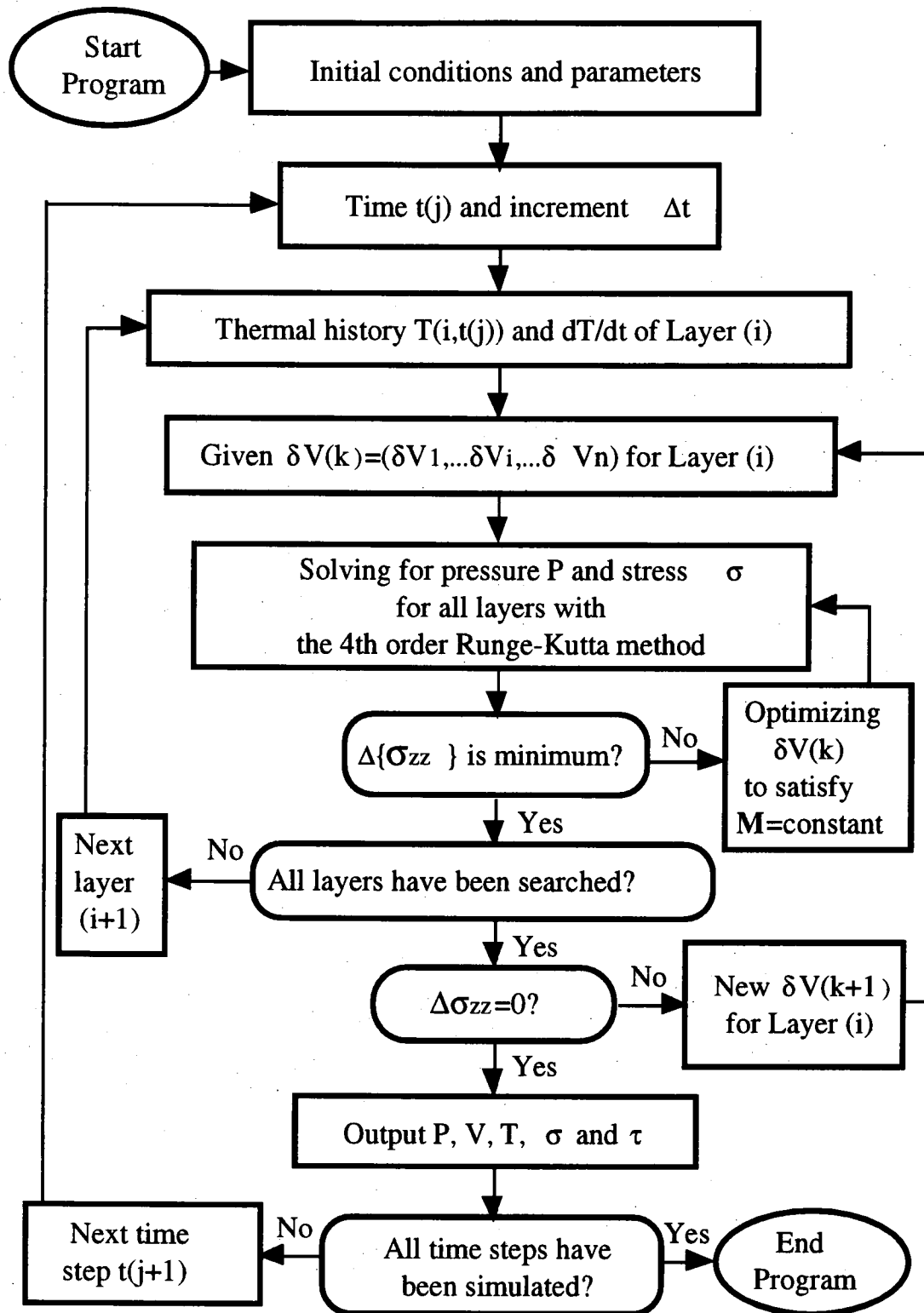


Figure 4.2-2. Programming chart-II for the cooling step

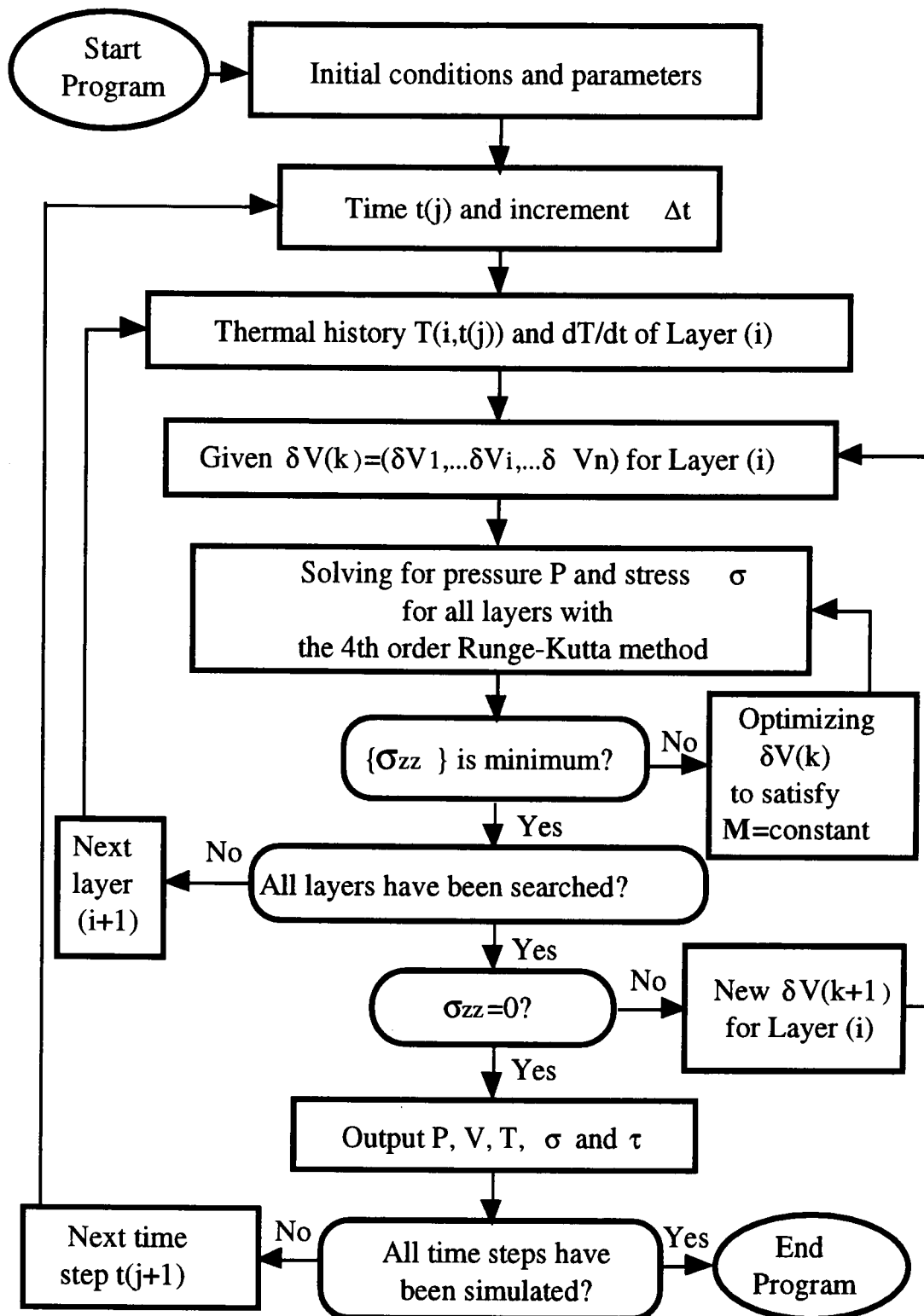


Figure 4.2-3. Programming chart-III for the post-ejection step

§4.3. Results and Discussion of Density-induced Residual Stresses in Injection Molding

Based on the theoretical work in the prior sections, several simulations of the post-filling steps in the injection molding were done on the computer. Three experimental injection molding cases from the literature[81][82][86] were studied. In this section, comparison of the simulations with the literature data will be made in terms of pressure, specific volume or density, and residual stresses. The results and discussion for density-induced residual stresses will now be presented. Also an alternate simulation of the post-ejection step will be discussed later in this section.

§4.3.1 Three Experimental Cases from the Literature

In the present work, simulation of three experimental cases from the literature were studied. These will now be reviewed.

Case I comes from the Cornell Injection Molding Program[86]. Case II is the work of a group at the Delft University of Technology[81]. Case III is the work of a group at the Eindhoven University of Technology[82]. The geometries used in these three cases are all rectangular slabs with very similar dimensions, as shown in Figures 4.3-1 and 4.3-2. There are two long dimensions in the x-y plane, and a short dimension in the z-direction. There are three pressure transducers in Case I, as shown in Figure 4.3-1 for tracing the experimental pressure, and four transducers in Cases II and III in Figure 4.3-2. Polystyrene from the Dow Chemical Company was employed in these experiments (Dow Styron 678U in Case I, Dow Styron 678E in Cases II and III). The melt temperature T_0 was 200 °C in all cases. The mold temperatures T_w were 32 °C for Case I, 50 °C for Case II and Case III. The initial packing pressures were 47.4 [MPa], 42.0 [MPa] and 78.0 [MPa]; the holding times were 16 seconds, 15 seconds, and 5 seconds; respectively.

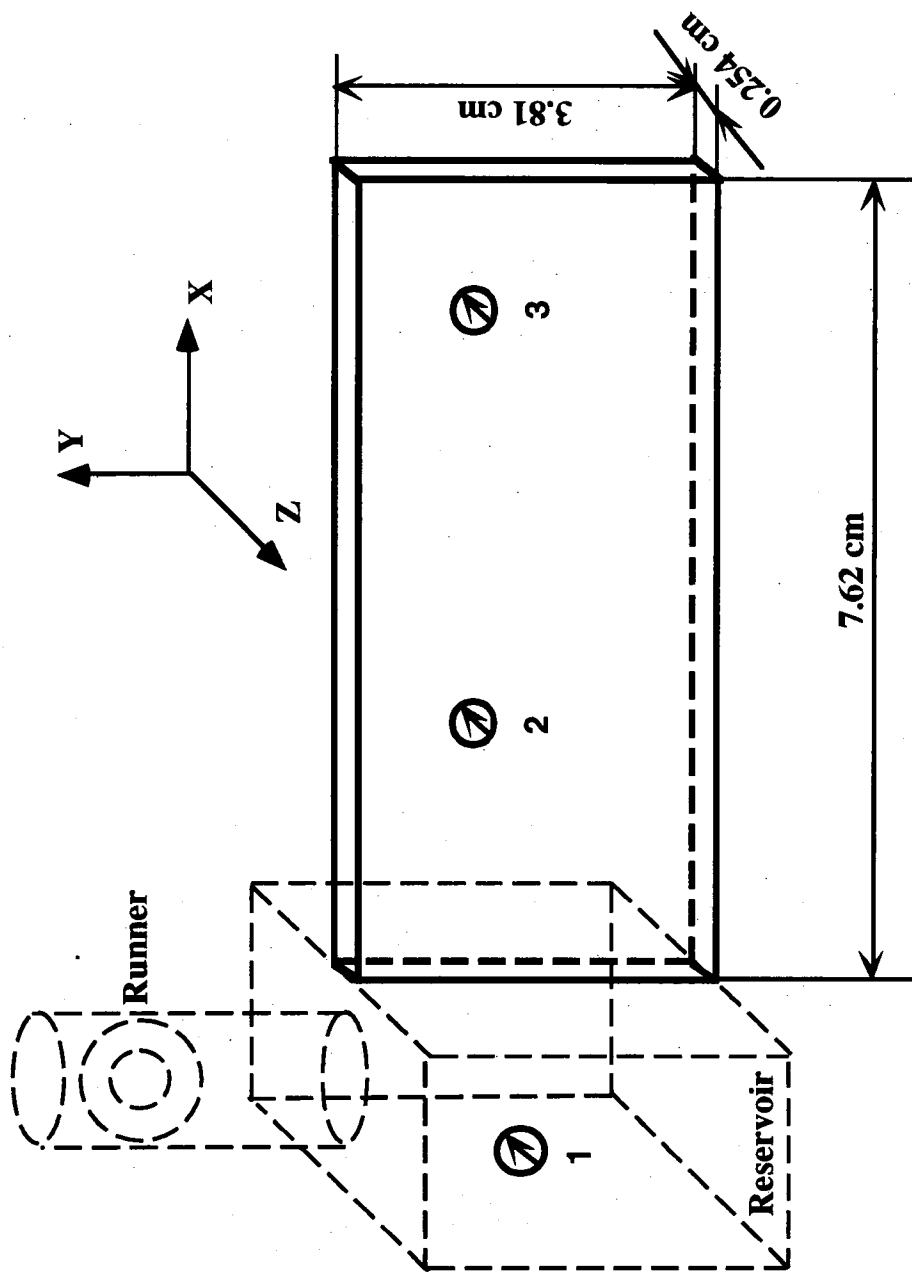


Figure 4.3-1 Schematic diagram of the geometry used at Cornell [86]

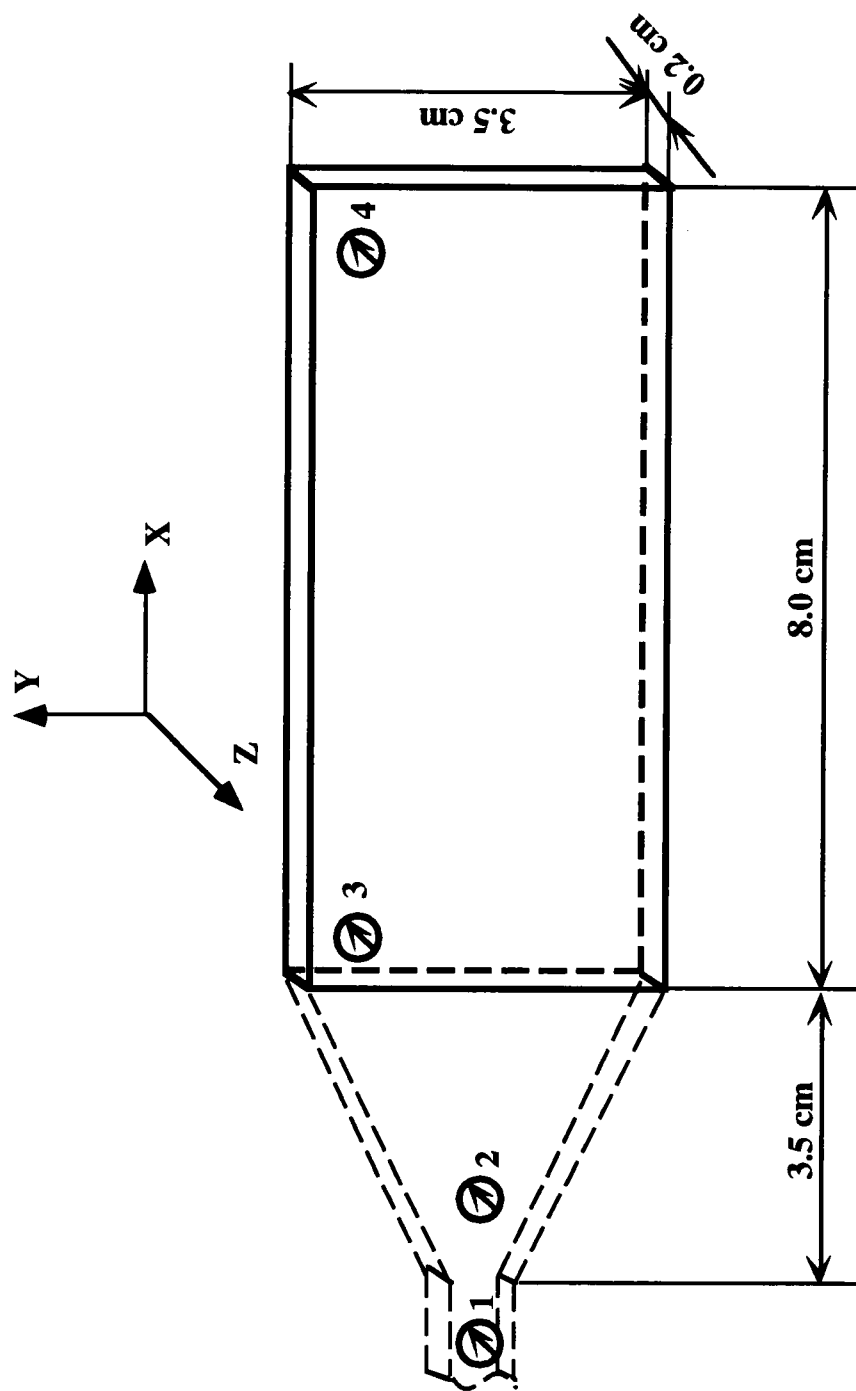


Figure 4.3-2 Schematic diagram of the geometry used by the Delft group[81] and Eindhoven group[82]

In the present work, the terminology for the packing and cooling steps is somewhat different from that in the literature. It is assumed that:

(1) the packing step starts at the end of the filling, and ends at the time at which the pressure at position 1 is almost constant (holding pressure), but the pressure at position 2 begins to decrease obviously in both Figures 4.3-1 and 4.3-2;

(2) when the packing ends, the cooling step begins; the cooling step continues until the part is ejected;

(3) some amount of extra mass is added to the cavity during the packing step only;

(4) during the cooling step, mass rearrangement occurs, but the movement takes place only in the z-direction;

(5) after the mold opens, one has the post-ejection step, although the temperature may still change during this step.

By these kinds of assumptions, the following values were estimated for the three simulations: the packing times were 2, 4 and 2 seconds, the cooling times were 14, 11 and 17 seconds, respectively, for Cases I, II and III. There was no post-ejection data available for Case I. The ejected parts were stored at -18°C in Case II and at room temperature (assumed to be 23°C) in Case III. Independent of the storage temperature, all measurements were assumed to be made finally at room temperature. Three cases are summarized in Table 4.3-1. The simulations of these cases will be discussed in the following sections.

§4.3.2 Temperature Profiles in the Injection Molded Slabs

As mentioned before, the energy (heat transfer) equation can be solved independently for the temperature profile in a solid slab. Since the present work simulated the three steps in injection molding starting from the end of filling, one has to deal with the

Table 4.3-1
Summary of the three experimental cases
(Cornell, Delft and Eindhoven groups)*

Step	Term [unit]	Case I		Case II		Case III	
		Cornell		Delft		Eindhoven	
Filling	Materials: Polystyrene (PS)	Dow Styron 678U		Dow Styron 678E		Dow Styron 678E	
	Melt Temperature [°C]	200		200		200	
	Mold Temperature [°C]	32		50		50	
Packing	Packing Time [sec]	2		4		2	
	Initial Packing Pressure[Pa]	4.74×10^7		4.2×10^7		7.8×10^7	
Cooling	Cooling Time [sec]	14		11		17	
Post-ejection	Storage Temperature [°C]	Not available		-18		23	

*The terminology for the packing and cooling steps is somewhat different from that in the literature, as explained in the text.

temperature distribution at the end of filling. Because some cooling already has taken place during filling, the temperature distribution at the end of filling affects the thermal history of the subsequent steps. In this work, Equation 4.4 was employed for the packing and cooling steps and Equation 4.11 for the post-ejection step due to the different conditions involved.

For obtaining the temperature distribution at the end of filling and determining the necessary parameters, the following procedures were carried out.

1. Under the conditions given for the three cases[81][82][86], the gapwise temperature profiles at the end of filling were read out of the C-MOLD program (from AC Technology, Ithaca, New York) for each case.

2. The transient heat transfer program (Equation 4.4, with an infinite heat transfer coefficient) was run starting from a time somewhat before time zero in the simulation (a "prior time"). It was assumed that the slab has an initial uniform temperature of 200 °C at time $t=0$ and the slab was in touch with the mold wall, i.e., the surface temperatures were kept at 32 °C for Case I, 50 °C for Cases II and III. The thermal diffusivity is constant, $\alpha = 7 \times 10^{-4}$ [cm²/sec], which was decided by k , ρ and C_v taken from the C-MOLD database.

3. A linear search procedure was employed in the calculations to determine the prior time for each case for which the temperature profiles obtained from the C-MOLD program were well matched by those from transient heat transfer theory (within 1 °C at the centerline).

4. The prior times determined from the above calculations were 0.8 [sec] for Case I, 0.2 [sec] for Cases II and III. Then, the transient heat transfer programs (Equation 4.4 with an infinite heat transfer coefficient) were used in the simulation to determine $T(i,t)$.

After the mold was opened, the parts are exposed to a different environmental condition (post-ejection step). One has to deal with their thermal histories in terms of a finite heat transfer resistance as discussed in Section §4.1.1. This work simulated the post-ejection step only for Cases II and III. The procedures to deal with the thermal history of this step are described below.

1. The transient heat transfer program (Equation 4.4, with an infinite heat transfer coefficient) was run with an initial uniform temperature of 200°C at time $t=0$. The surface temperature was taken same as the wall temperature, i.e., 50°C for Cases II and III. The prior time for each case was determined by the procedures described above. One obtained temperature profiles by running these programs until the end of the cooling (when the mold opened—that is, the starting of the post-ejection step).

2. One runs another transient heat transfer program (Equation 4.11 with a finite heat transfer coefficient) with an arbitrary uniform temperature at time $t=0$, namely, 70°C for both cases. This new time $t=0$ and the uniform temperature correspond to the start of the post-ejection step. The surface temperatures were determined by the storage environmental conditions, -18°C for Case II and 23°C for Case III.

3. There is also a new “prior time” for the post-ejection step, such that the temperature profiles at the end of cooling obtained from the first step (Equation 4.4 with an infinite heat transfer coefficient) were well matched by these calculations (Equation 4.11 with a finite heat transfer coefficient). By this means, the temperature profiles are almost continuous for times before and after the mold opens (within 1°C at the center line). The new “prior times” for the post-ejection step were 10.65 in Case II and 14.28 seconds in Case III.

4. The heat transfer coefficient h_{tc} was determined by fitting the cooling experiments of the present work (Chapter 3) with Equation 4.11, which gave $h_{tc}=7\times 10^{-3} [\frac{W}{cm^2 \circ K}]$. The arbitrary uniform temperatures and prior times determined by these calculations were used in the simulations for the thermal histories during the post-ejection step.

The temperature profiles (thermal histories) obtained by the above procedures for the simulations are reported in Figures 4.3-3, 4.3-4 and 4.3-5.

§4.3.3 Pressure Profiles during Packing and Cooling: Comparison of Case I with Literature Data

§4.3.3.1 Complete Simulation

As shown in Figure 4.3-1, three pressure transducers are located along the x-direction, positions 1, 2 and 3, namely. The pressure (total pressure, $-\sigma_{zz}$) measured by the Cornell group[86] shows obviously that there is a pressure gradient along the flow direction. However, in the present simulation, it was assumed that in the x-y plane the pressure and also the temperature are uniform and similar to that at position 3. A prescribed pressure function formed from literature data[86] was imposed during the packing step. The pressure decrease during the cooling step was predicted, not imposed.

For simulation of this case, the reference conditions are that $T_0=T_s=200\text{ }^\circ\text{C}$ and P_0 at atmospheric pressure; thus, $V_0=1.034\text{ [cm}^3\text{/g]}$. The wall temperature of the mold is $T_w=32\text{ }^\circ\text{C}$. The packing and cooling times are 2 and 14 [sec], respectively. The equilibrium glass transition temperature $T_{ge}=85\text{ }^\circ\text{C}$ was used at P_0 [1][5]. The glass transition temperature $T_g(P)$, the pressure compressibility

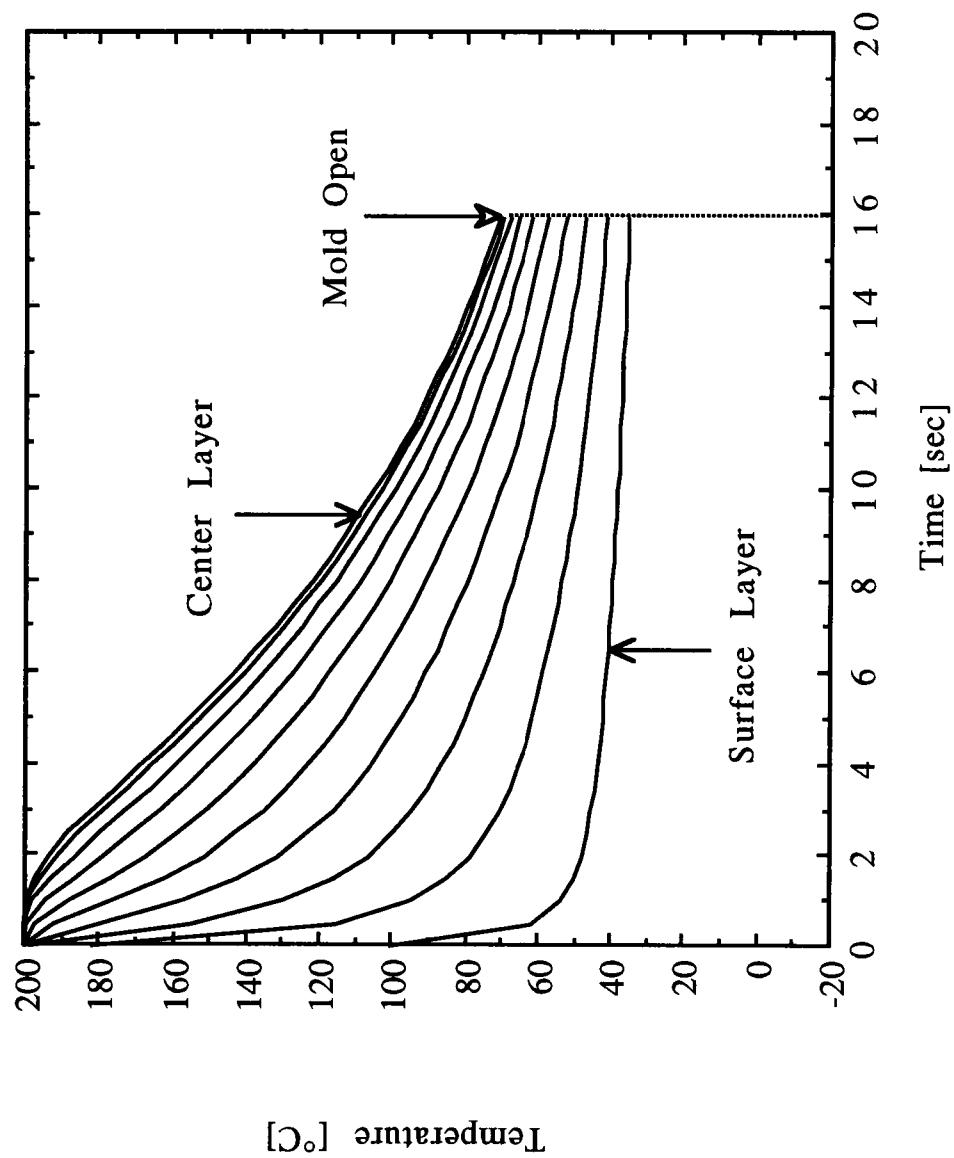


Figure 4.3-3 Temperature profiles calculated by Equation 4.4 for Case I

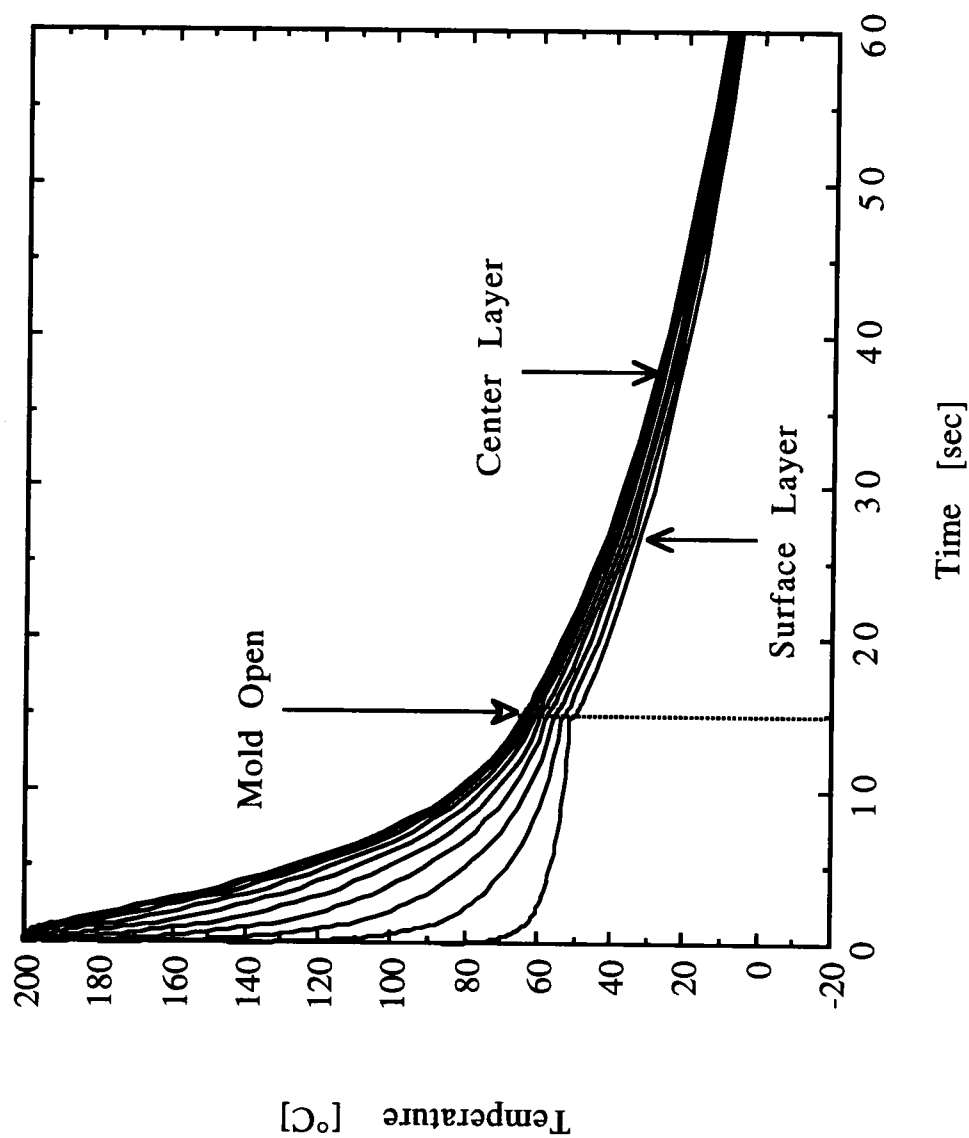


Figure 4.3-4 Temperature profiles calculated by Eqs. 4.4 and 4.11 for Case II

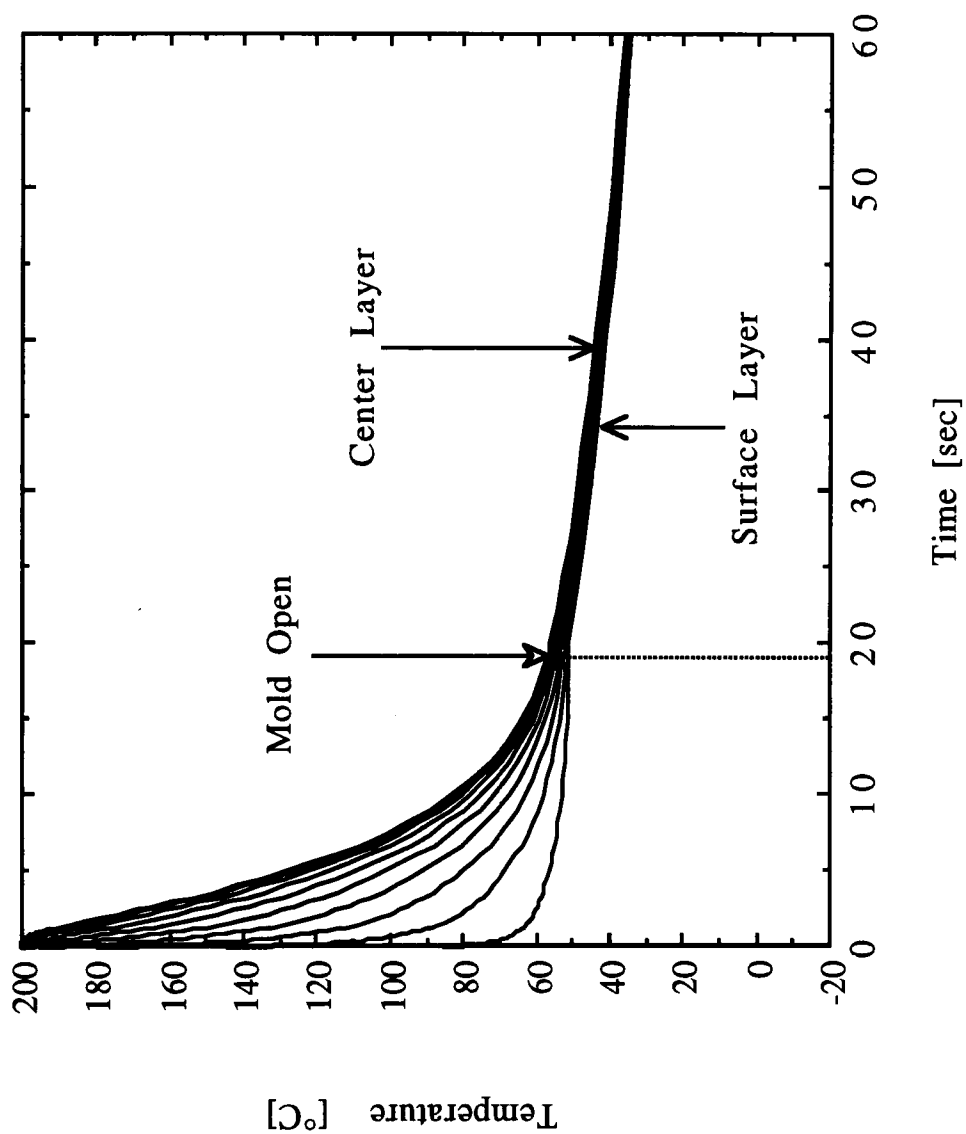


Figure 4.3-5 Temperature profiles calculated by Eqs. 4.4 and 4.11 for Case III

coefficients, κ_r and κ_g , the thermal expansion coefficients, α_r and α_g , are pressure and temperature-dependent given in the literature[79]. In this research, only constant values of α_r , α_g , κ_r and κ_g , were selected to simplify the program and to reduce simulation time. The coefficients, α_r , α_g , κ_r and κ_g were determined by fitting the data of Oels and Rehage[79] with a Tait type PVT equation[89]. The values of these coefficients are $\alpha_r=5.8 \times 10^{-4}$ [1/°K], $\alpha_g=2.3 \times 10^{-4}$ [1/°K], giving $\alpha_a \approx 2.5 \times 10^{-4}$ [1/°K]; $\kappa_r=9.3 \times 10^{-10}$ [1/Pa] and $\kappa_g=5.3 \times 10^{-10}$ [1/Pa], giving $\kappa_a \approx 7.3 \times 10^{-10}$ [1/Pa]. A linear equation for $T_g(P)$ was employed. This equation reads as

$$T_g(P) = T_{ge} + C_{Tg}P(t) \quad (4.58)$$

where $C_{Tg}=3.3 \times 10^{-7}$ [°C/Pa]. The time constant at a reference state T_0 and P_0 is $\tau_0=1.81 \times 10^{-8}$ [sec]. As described in Chapter 3, the constant $-\beta$ was set at 500. The adjustable constant n was rate-dependent. For convenience a linear equation instead of the tabulated numbers was used to determine n :

$$n = n_0 - C_n \log(-q) \quad (4.59)$$

where q is the cooling rate in [°C/sec], $n_0=0.80$, and $C_n=0.033$.

Regarding the anisotropic stresses, the second time constant for the stress relaxation (τ_{G0}) was obtained from the data of Racin[90] at a reference temperature of 160 °C as $\tau_{G0}=0.147$ [sec]. This time constant needs to be adjusted to the transient temperature at which the stresses are considered (Equation 4.26). Because the present simulations involve a large range of temperature scale and to avoid numerical overflow on the computer, two shift factor equations were made to cover the different temperature regions. For the higher temperature region, between 125 °C to 200 °C, a WLF equation was used with a reference temperature at $T_r=160$ °C, that is,

$$\log(a_G) = \frac{-c_1(T-T_r)}{c_2+(T-T_r)} \quad (4.60)$$

where $c_1=4.3$ and $c_2=80$ °C. For the lower temperature region, below 125 °C, an exponential type of shift equation was adopted with the same reference temperature at $T_r=160$ °C.

$$\ln(a_G) = -c_3(T-T_r) \quad (4.61)$$

where $c_3=0.22$ [1/°C] which lets the time constant $\tau_G(t)$ have a smooth connection at the temperature of 125 °C. As discussed in Section §4.1.2, the elastic modulus $G(t)$ is assumed to be temperature-dependent only. For the lower temperature region, $T(t)<80$ °C, $G(t)\equiv 1.5\times 10^9$ [Pa]; for the higher temperature region, $T(t)>120$ °C, $G(t)\equiv 0.2\times 10^6$ [Pa]; for the temperature between 80 °C to 120 °C, an empirical equation corresponding to the temperature was chosen and to be used in the simulations:

$$G(T(t)) = -98959 + 3245T - 34.89T^2 + 0.1226T^3 \quad 80\text{ °C} < T(t) < 100\text{ °C} \quad (4.62)$$

$$G(T(t)) = 10^{(652 + 16.96T + 0.15T^2 - 0.00044T^3)} \quad 100\text{ °C} < T(t) < 120\text{ °C} \quad (4.63)$$

This continuous elastic modulus profile is shown in Figure 4.1-2.

A prescribed packing pressure was imposed during the packing. The pressure data at the point 3 taken from the literature[86] were fitted by a polynomial equation $P_{\text{pack}}(t)$ and used in the simulation program. It reads

$$P_{\text{pack}}(t) = (46.6 + 2.5035t - 1.773t^2 + 0.16145t^3 - 0.0044t^4) \times 10^6 \quad (4.64)$$

where t is the time in seconds and $P_{\text{pack}}(t)$ in [Pa].

A fourth-order Runge-Kutta method was employed for solving the simultaneous differential equations, Eqs. 4.55—4.57. The combination of the optimum techniques using linear and multimodal search procedures was employed as discussed in Section §4.2. The simulation continued for 16 seconds to predict the total pressure during the cooling step. The optimum procedure requires setting a pre-selected criterion near zero to terminate the iteration steps; this near zero value was taken to be 1×10^5 [Pa]. The optimum objective was set for the total pressure ($-\sigma_{zz}$) in the z-direction:

- (1) The total pressure in the z-direction was equal to the prescribed packing pressure during the packing, Equation 4.33;
- (2) There was no total pressure gradient in the z-direction during the cooling, Equation 4.31.

The pre-selected (“almost zero”) criterion for evaluating the optimization objective was 1×10^5 [Pa]. Typically, the initial packing pressure is of the order of 1×10^7 [Pa]. By defining a relative error as the summary of the difference of the total stress over the initial packing pressure, this pre-selected criterion means that the relative error of the total stress is less than 1%. This criterion was examined and satisfied for each time step. The pre-set criterion for evaluating the satisfaction of the constant volume (or the constant mass) was 5×10^{-6} . This pre-set criterion gives a limit of error of density within 5×10^{-6} [g/cm³]. The criterion was examined and satisfied for every optimum search. The number of iterations was set at 30 in the present work. If the criteria were matched before the iteration reached the limitation of 30, the program automatically shifts to next time step for a new iteration of the optimization; otherwise, the program is forced to shift to the next time step after 30 iterations. It needs to be realized that if this situation occurs, it means that the criteria are not matched in that iteration. The simulation can continue smoothly but slowly. The criteria may be matched in the later iterations and the optimization may succeed finally. However, the error of the simulation may be larger than the limitation

mentioned above. The computer program is presented in Appendix A. The comparison of the prediction with the literature data will now be presented.

As shown in Figure 4.3-6, the prediction of the total pressure fits the literature data very well. It indicates that volume-induced residual stresses must be given a great consideration in the simulation of the injection molding. In other words, the time-dependent density changes (non-equilibrium density) are playing an important role in injection molding.

§4.3.3.2 Two "Equilibrium" Simulations

Prior to the present work and the work of Ko and Bogue, investigators have always used an equilibrium PVT equation, not a time-dependent PVT as in the previous simulation. In order to compare these two frameworks (the equilibrium and the time-dependent equations), two equilibrium simulations of Case I were executed on the computer. These two simulations were based on the two different equilibrium conditions: one was the actual PVT data of Oels and Rehage[79], and the other was a shifted model (described by the Cornell group) which has a shifted specific volume line[87].

The experimental data of Oels and Rehage were obtained at various fixed pressures with a cooling rate of 0.005 [°C/sec]. Data at this very low rate are taken to be equilibrium ones. These data can be well fitted by an equilibrium PVT equation, such as the 2-domain Tait model with $T_{ge}=87.2$ °C. Figure 4.3-7 is a PVT plot of these data and the best fit by the group of the Cornell University[87]. This was used in the first equilibrium simulation.

In practice, a typical average cooling rate in injection molding is about 10 [°C/sec]. This cooling rate is much higher than that rate in the experiments of Oels and Rehage. It is hard to get a reasonable result in a simulation involving a high cooling rate by simply using

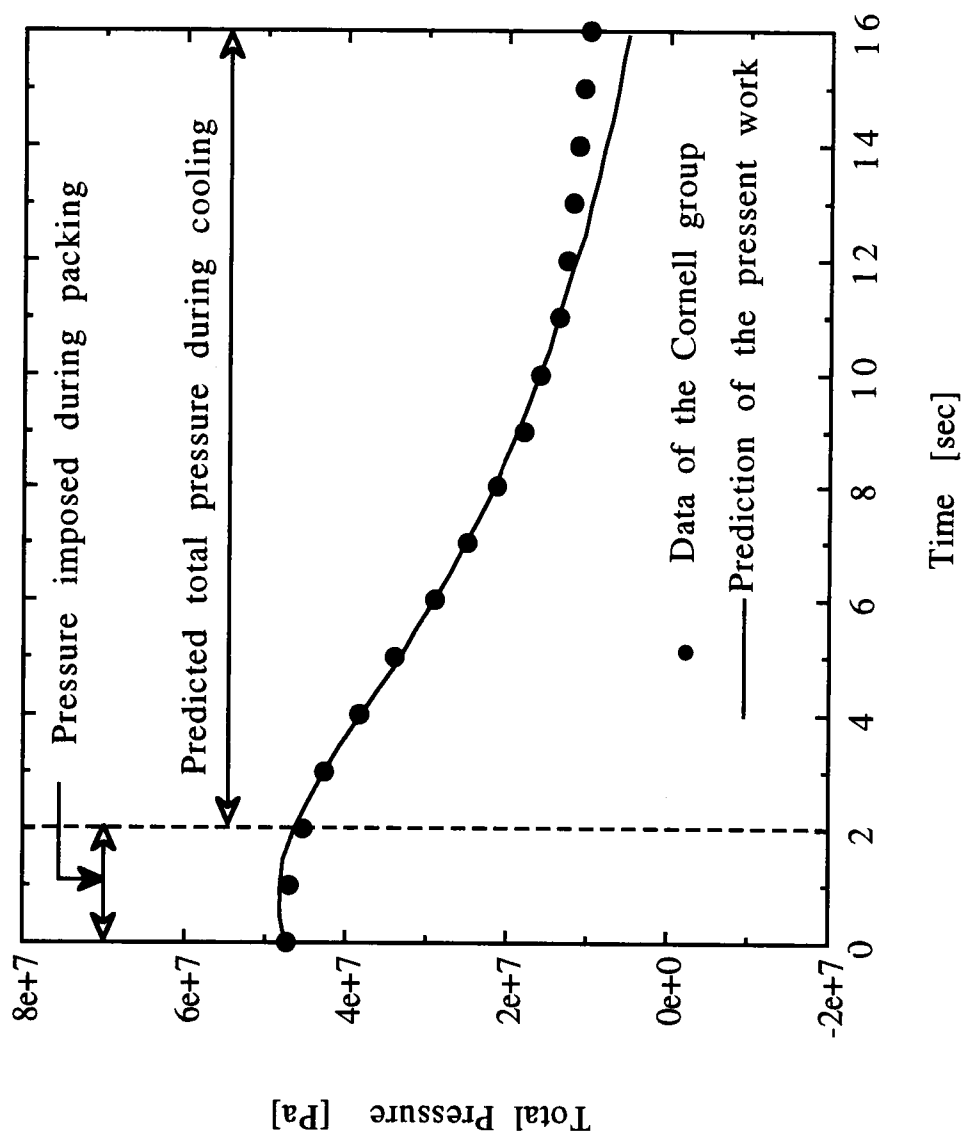


Figure 4.3-6 Comparison of the total pressure profile predicted by the non-equilibrium formulation with the data of the Cornell group

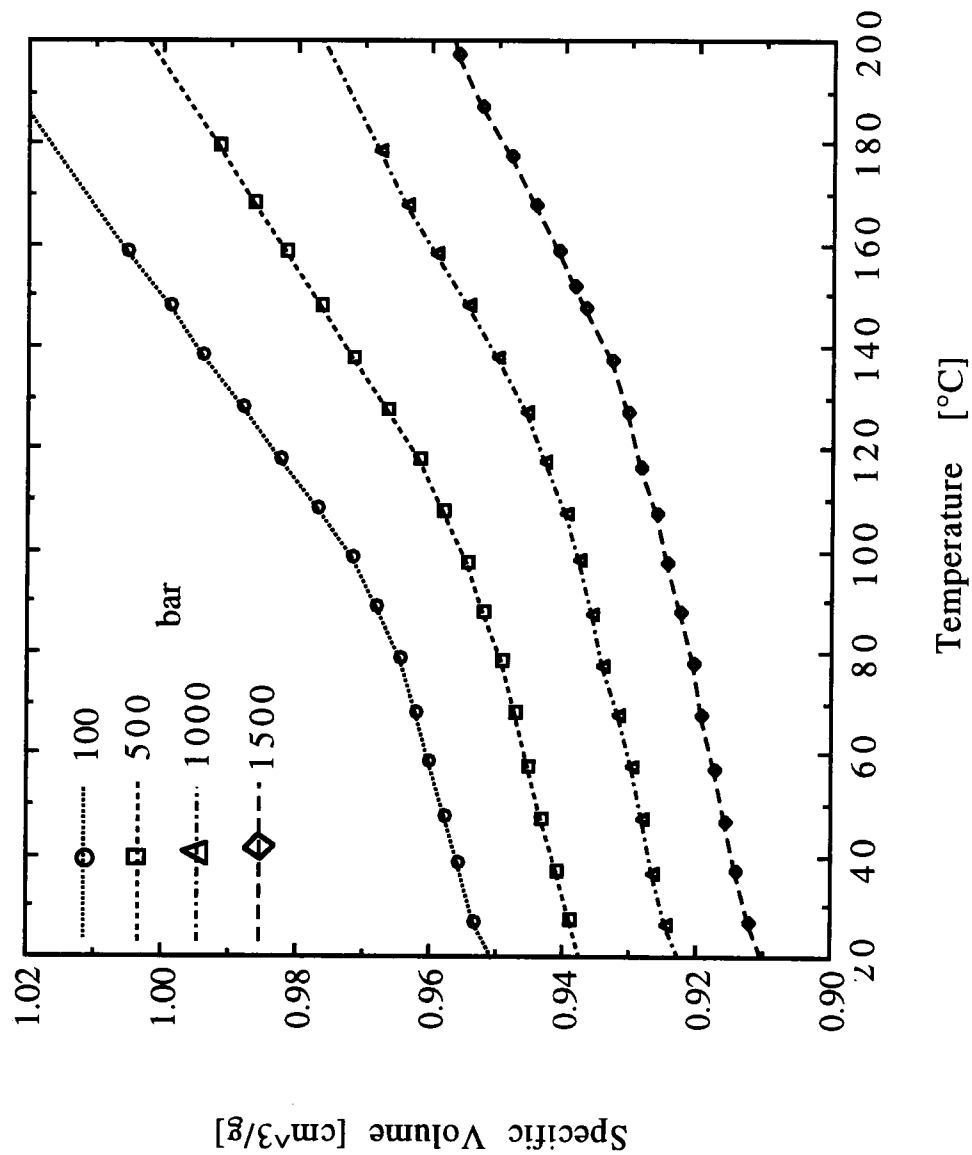


Figure 4.3-7 A PVT plot of the data (symbols) of Oels and Rehage[79] and the best fits (lines) with an equilibrium model $T_{ge}=87.2$ °C by the group at the Cornell University[87].

an equilibrium model without any adjustments, because the equilibrium PVT equation is only applicable for cases with very low cooling rates. In other words, one has to have some adjustable parameters in an equilibrium model to correspond the high cooling rate effects. The group of the Cornell University have also noted the effects of a high cooling rate. In order to account for the rate effects in the equilibrium framework, they have proposed a shifted model of T_{ge} of 103 °C. Figure 4.3-8 is a PVT plot of the shifted model taken from the work of the Cornell group[87]. By applying the shifted $T_{ge}=103$ °C, instead of the equilibrium $T_{ge}=87.2$ °C, they were able to demonstrate that a high cooling rate effect has approximately been accounted for in the injection molding simulation. This shifted model was used in the second equilibrium simulation.

To run these two equilibrium simulations on the computer, one has to select an appropriate time constant. The first simulation used a very small time constant, $\tau \ll 1$ [sec] and an equilibrium glass transition temperature T_{ge} of 87.2 °C, which is associated with to Figure 4.3-7. The reason for selecting the time constant $\tau \ll 1$ [sec] (but not $\tau=0$) is that one has to choose a small number to approach the equilibrium condition; meanwhile, the number must be "large" enough to allow the program to run on the computer without an overflow problem—that is, it must be much bigger than the lowest numerical limit of the computer. The typical values for the time constant τ were in the range from 1×10^{-5} [sec] to 5×10^{-2} [sec]. The second simulation also used a very small time constant (same as that used in the first simulation) but with a shifted glass transition temperature T_{ge} of 103 °C at the reference atmospheric pressure, which corresponds to Figure 4.3-8.

To look at the importance of the non-equilibrium (time-dependent) density changes, a comparison of these results from the equilibrium simulations with that from the complete simulation and the data from the literature was made to help to understand the importance of the non-equilibrium (time-dependent) density

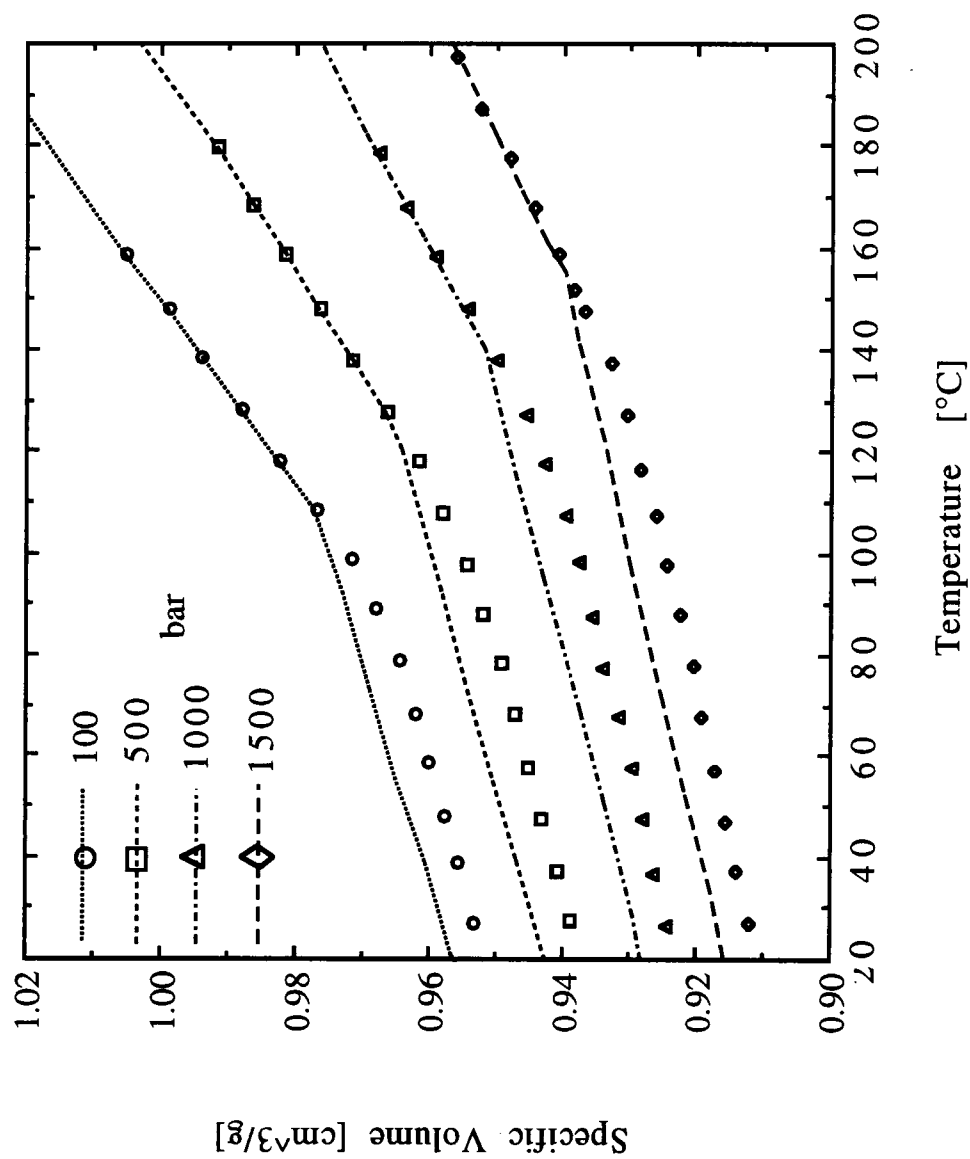


Figure 4.3-8 A PVT plot of the data (symbols) of Oels and Rehage[79] and the best fits (lines) with a shifted model $T_{ge}=103$ °C by the group at the Cornell University[87].

changes. The comparison will be given in the next section.

§4.3.3.3 Comparison of Simulations

The total pressure profiles predicted by the two equilibrium simulations are presented in Figure 4.3-9 with the data from the literature and the prediction from the non-equilibrium simulation in the prior section. As expected, the predictions from the equilibrium simulations are not in agreement with the literature data.

It can be seen from the figure that the first equilibrium approach, ($T_{ge} = 87.2$ °C), gives an unusual pressure peak during the cooling. The unusual large pressure peak shown by the dashed line (marked as Equilibrium) can be explained in the terms of PVT state changes. Remember that the temperature has been dealt with independently in the simulations, thus, it is a pressure-volume problem. Also during the cooling, the total volume is a constant (the volume of the cavity) and the pressure has to change so that this constraint condition can be satisfied. However, the PVT relationship is a very complicated one because of the discontinuity in the pressure compressibility coefficients and the thermal expansion coefficients. They change their values when the temperature passes through the glass transition temperature.

The lower pressure peak shown by the dashed and dotted line (marked as Shifted model) comes from the Cornell shifted model. This is an equilibrium approach with T_{ge} shifted to 103 °C. The magnitude of the peak is reduced significantly. The better prediction by the shifted model is understandable. According to the present work in Section §3.3, Figure 3.3-7, $T_{ge}=103$ °C corresponds to a cooling rate of about 10 [°C/sec]. This rate is on the typical order of an average cooling rate in injection molding. Obviously, $T_{ge}=103$ °C is an apparent T_g (rate-dependent)—that is, a non-equilibrium condition. That means some non-equilibrium density (time-dependent) has been built into the model when a shifted T_{ge}

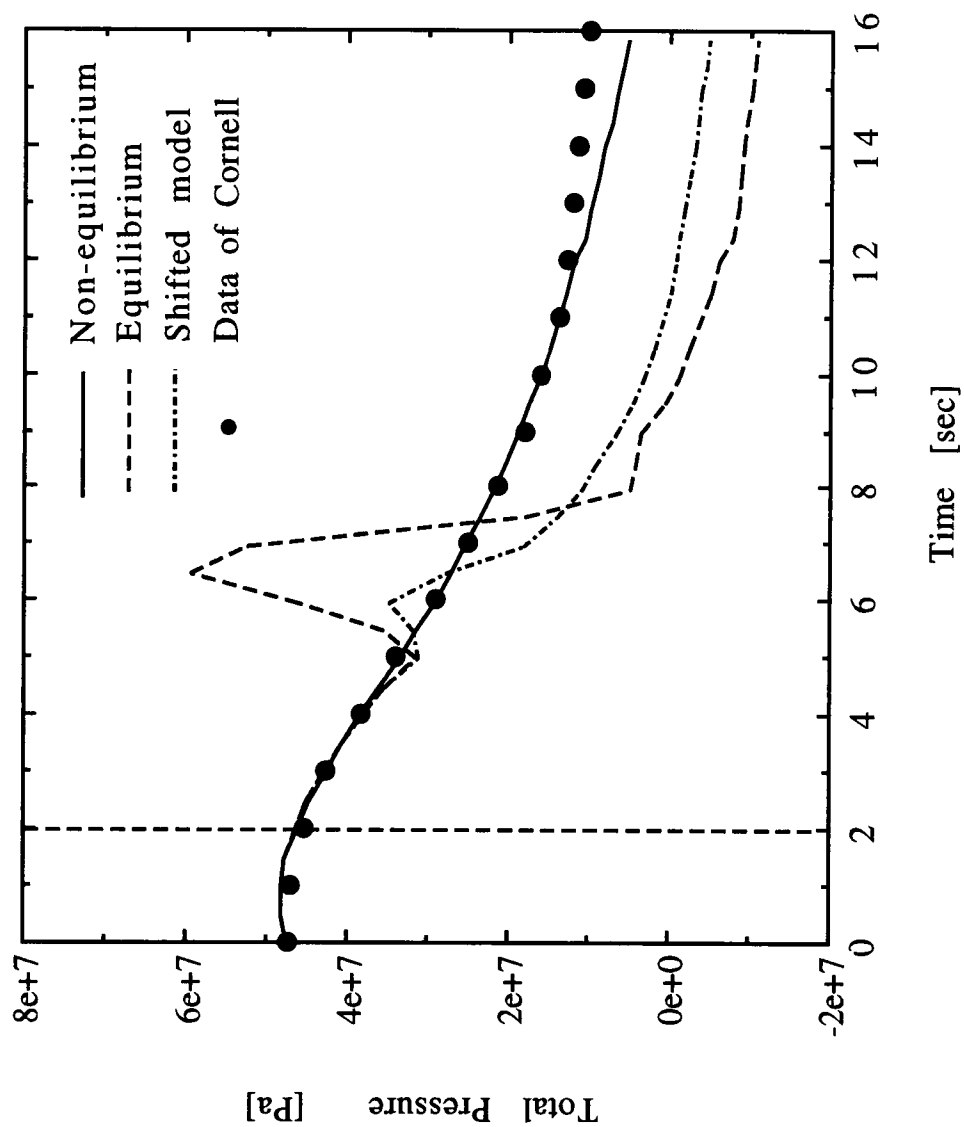


Figure 4.3-9 Comparison of the total pressure profiles predicted by the non-equilibrium formulation, equilibrium approaching and shifted model with the data of the Cornell group

is adopted. That explains why the shifted model improves the prediction. In the actual injection molding, the cooling rates are not a constant, the rates vary with time and position. Thus, simply using a shifted parameter in an equilibrium model, such as $T_{ge} = 103\text{ }^{\circ}\text{C}$, is not good enough to simulate such a complicated problem.

Finally, from these comparisons, it can be concluded that the time-dependent density changes play an important role in the situation in which a high cooling rate involves, such as in injection molding. Thus, an appropriate non-equilibrium framework is necessary. The studies of Case I show that the theoretical work of this work (in Sections §4.1 and §4.2) is applicable.

§4.3.4 Simulations of the Two Cases Involving Different Injection and Post-ejection Histories

In this section, the non-equilibrium formulation were applied to all three steps in injection molding. Cases II and III with various injection and post-ejection histories were simulated. There will be presented now.

§4.3.4.1 The Literature Data and the Simulation Procedures

As shown in Figure 4.3-2, there are four pressure transducers located along the x-direction, positions 1, 2, 3 and 4. It also assumed in the simulation that the pressure and the temperature in the x-y plane are uniform and similar to that at position 3, which is a typical position. The parameters and constants to be used in the non-equilibrium simulations for Cases II and III were the same as that used in Case I. Also, those equations, from Eq. 4.58 to Eq. 4.63, are still valid here. The differences in Cases II and III involve small changes in the dimensions and in the injection and post-ejection histories. For Cases II and III, the injection temperature is $T_0 = T_s = 200\text{ }^{\circ}\text{C}$; the mold temperature is $T_w = 50\text{ }^{\circ}\text{C}$. The packing times

were estimated as 4 and 2 seconds; the cooling times were estimated as 11 seconds and 17 seconds; the post-injection storage temperatures were $-18\text{ }^{\circ}\text{C}$ and $23\text{ }^{\circ}\text{C}$; and the initial packing pressures were 4.2×10^7 [Pa] and 7.8×10^7 [Pa], respectively. These are shown in Figure 4.3-2 and Table 4.3-1.

The measurements of Case II done by the group at the Delft University of Technology[81] can be summarized as follows:

(1) The total pressure in the z-direction was traced by transducers during the packing and cooling;

(2) The anisotropic stresses in the x-direction were measured by a layer removal method at room temperature (the parts were molded and ejected, then, stored in the condition of $-18\text{ }^{\circ}\text{C}$ for an unstated time before measurement).

These data are shown in Figures 4.3-10 and 4.3-11.

The measurements of Case III done by the group at the Eindhoven University of Technology[82] can be summarized as follows:

(1) The total pressure in the z-direction was traced by transducers during the packing and cooling;

(2) After the parts were molded and ejected, they were cut into small pieces. The specimens were put into DGC. The gapwise density distribution data were taken after aging for two and nine days (the parts were assumed to be stored and measured at $23\text{ }^{\circ}\text{C}$).

These data are shown in Figures 4.3-12 and 4.3-13.

The functions of the prescribed packing pressure which were imposed during the packing steps were formed by fitting the pressure data taken from Cases II and III at position 3. These data were fitted with polynomial equations and applied in the simulations. Two equations read as

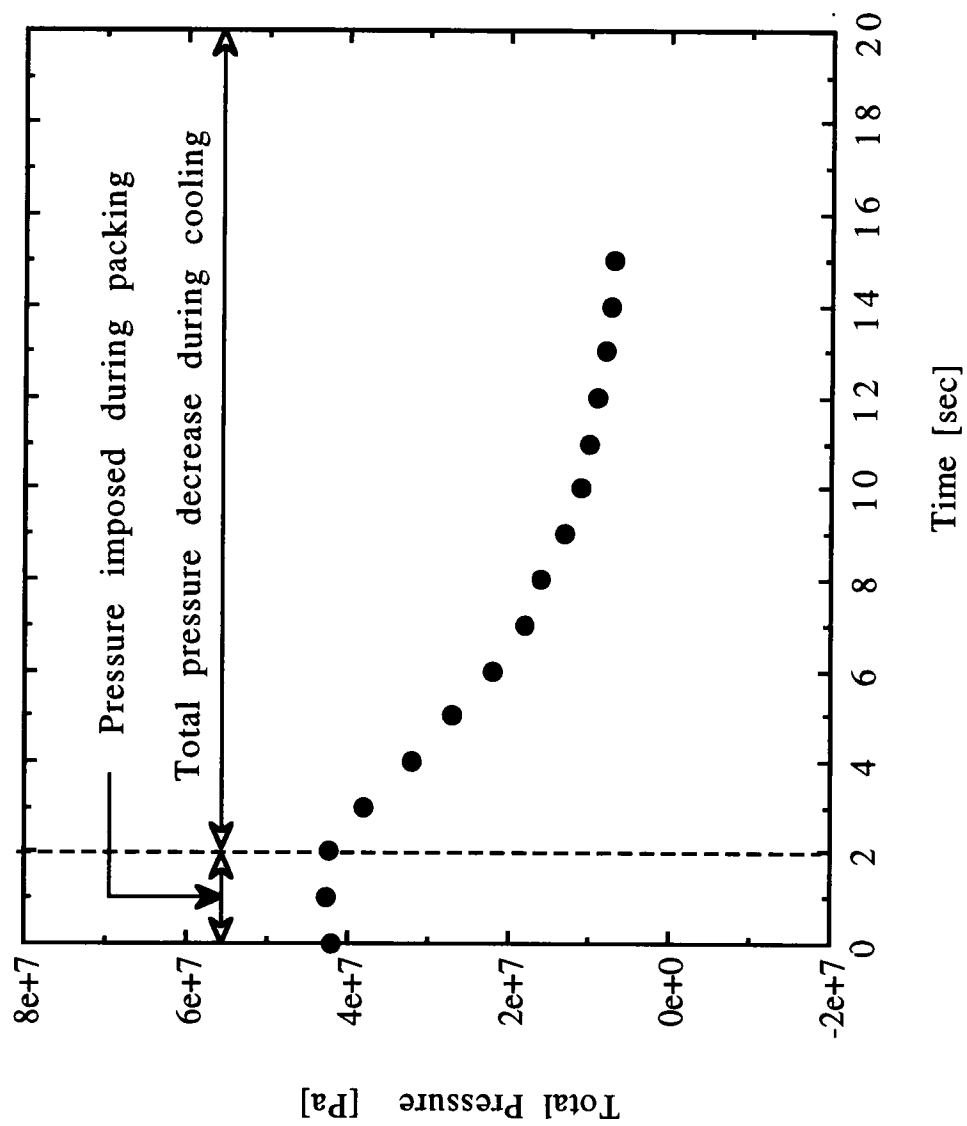


Figure 4.3-10 Data of the total pressure measured by the group at the Delft University of Technology[81]

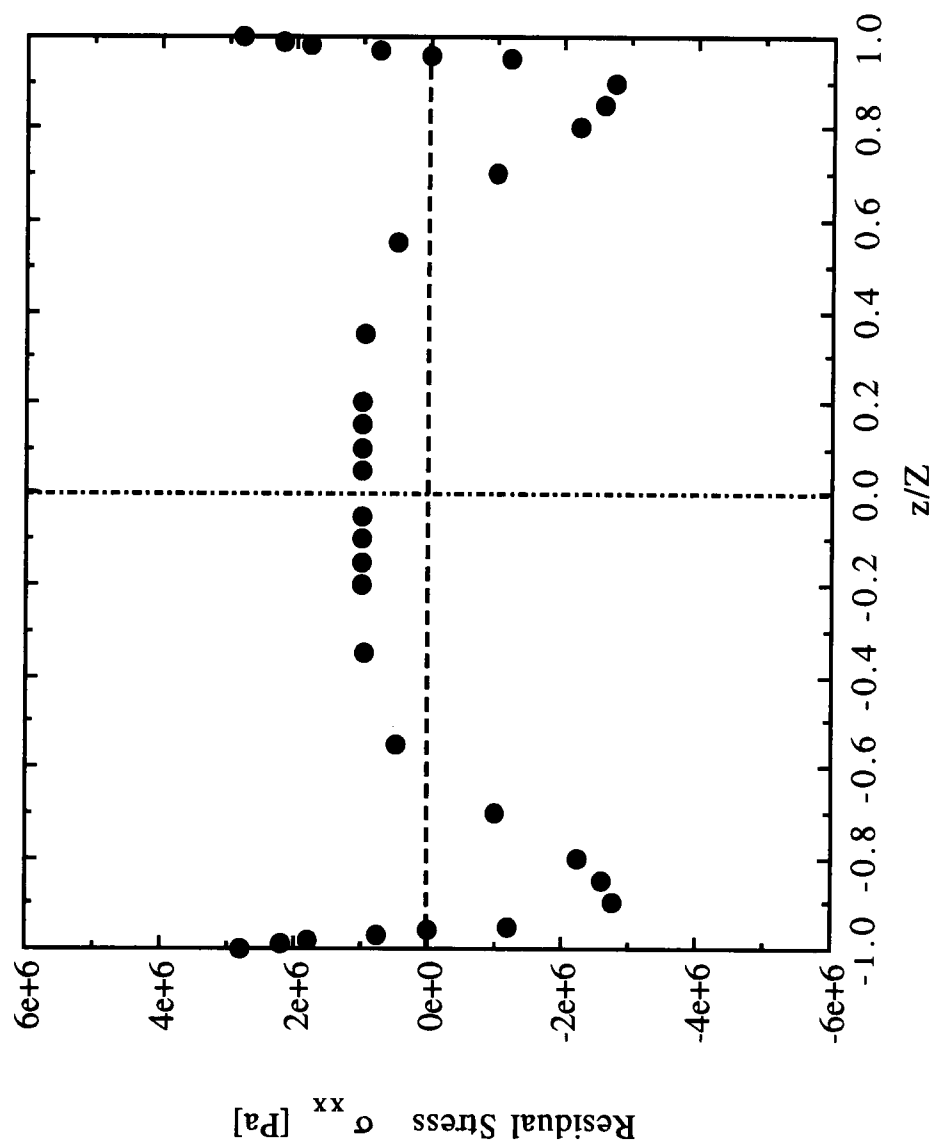


Figure 4.3-11 The data of the residual stresses measured by the group at the Delft University of Technology[81]

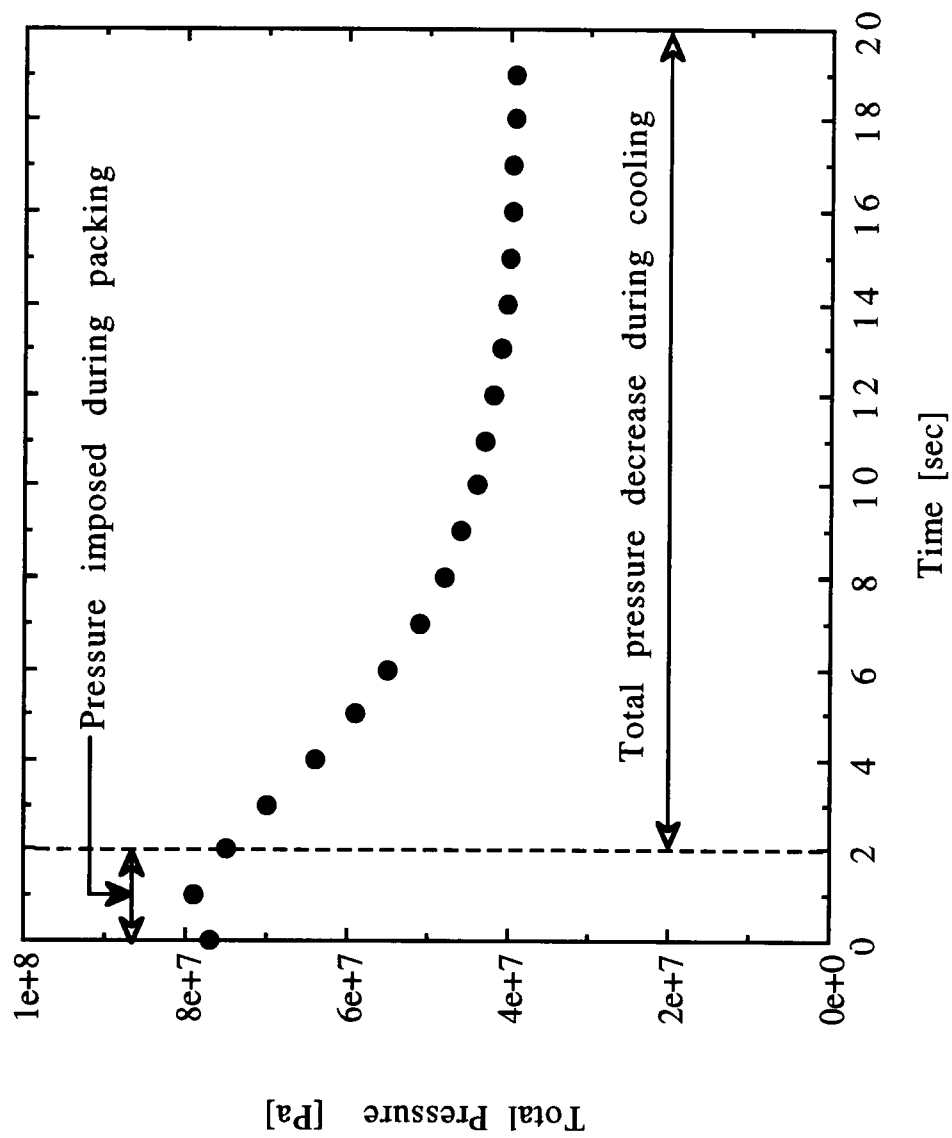


Figure 4.3-12 The data of the total pressure measured by the group at the Eindhoven University of Technology[82]

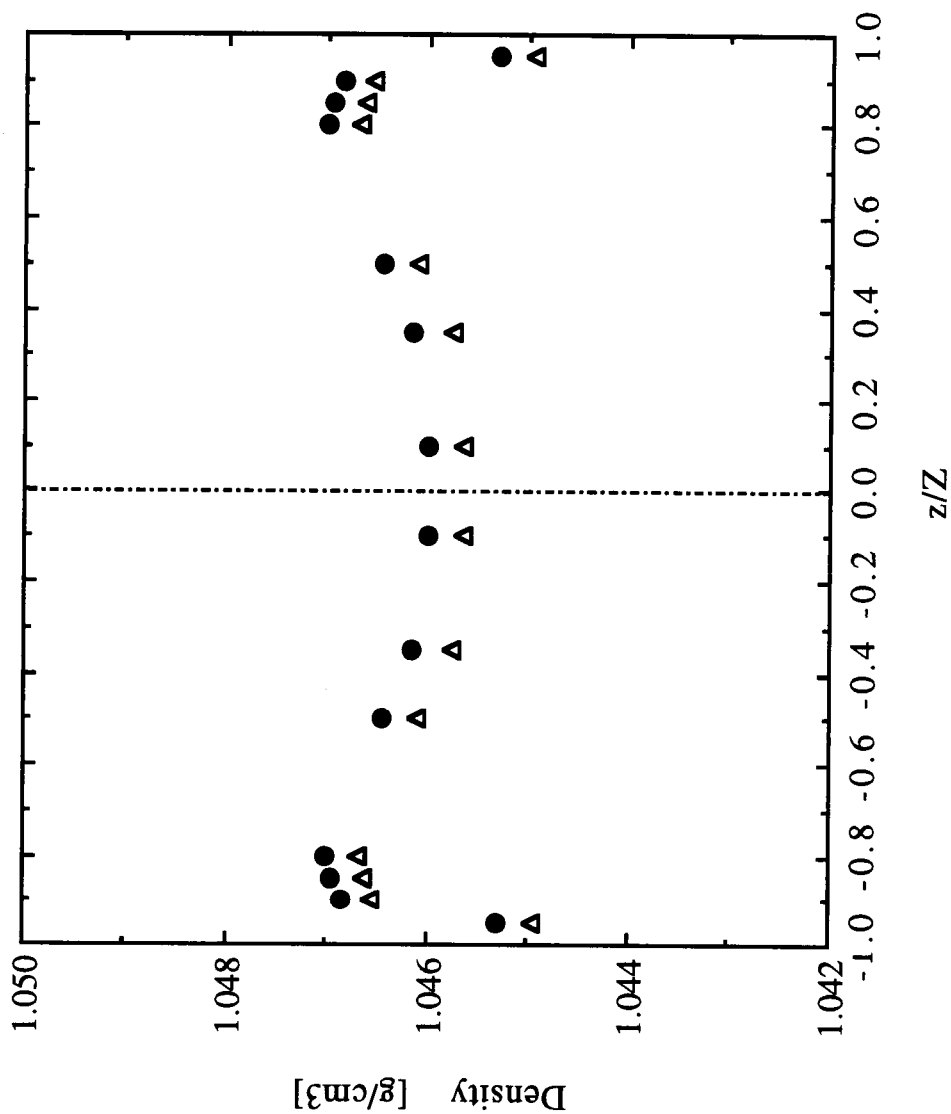


Figure 4.3-13 Gapwise density distribution measured by the group at the Eindhoven University of Technology[82]
 Δ Aging for 2 days; $\bullet$ Aging for 9 days.

$$P_{\text{pack}}(t) = (42 + 2.5035t - 1.773t^2 + 0.16145t^3 - 0.0044t^4) \times 10^6 \quad \text{Case II} \quad (4.65)$$

$$P_{\text{pack}}(t) = (77.13 + 4.77t - 3.865t^2 + 0.578t^3 - 0.00283t^4) \times 10^6 \quad \text{Case III} \quad (4.66)$$

where t is the time in [sec] and $P_{\text{pack}}(t)$ in [Pa]. The mathematical method, optimum techniques and search procedures employed here were the same as that in the complete simulation (Case I) in the previous section. The simulations continued and covered all of the three steps in injection molding. The optimum objectives for the packing and cooling steps were the same as that used in Case I. The optimum objective for the post-ejection step was that the applied pressure throughout the part was atmospheric, Equation 4.35. The criteria used in the previous section were similar in principle for all three steps, but the numerical values are different: 1×10^5 [Pa] for the packing and cooling steps and 100 [Pa] for the post-ejection step. The computer programs are presented in Appendices B and C. The results and comparison will now be presented.

§4.3.4.2 Pressure Decrease and Residual Stresses: Comparison of Simulation with Case II

Figure 4.3-14 is a plot of the predicted total pressure of Case II, $-\sigma_{zz}$, and the same literature data as that in Figure 4.3-10. This figure shows that, as expected, the prediction agreed well with the literature data.

The total stress in the z -direction, σ_{zz} , is composed of two components, isotropic stress $-P$ (isotropic pressure P) and anisotropic stress σ'_{zz} (Equation 4.22). The meaning of the terms of isotropic here is that the component P is isotropic throughout each layer at a given time; it may be isotropic throughout the whole part at some times (such as that at the end of the filling, by assumption), but it is

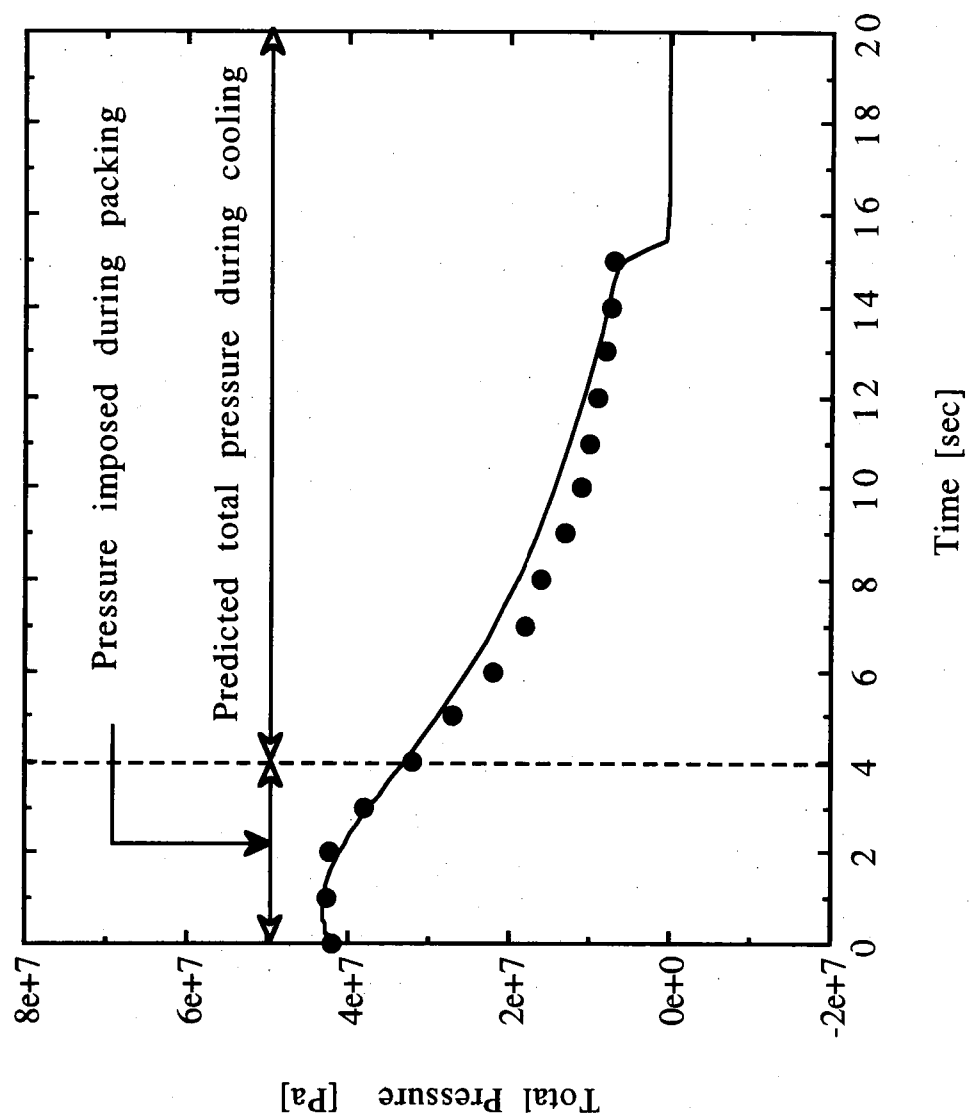


Figure 4.3-14 Comparison of the total pressure for Case II;
 — Prediction of the present work, • Data of the Delft Group

not necessarily always so. It varies with time and position. The present formulation is able to predict all these components at various times and positions, as well as the density distributions.

Figure 4.3-15 is a plot of the gapwise profiles of the isotropic pressure P (negative of the isotropic stress), at several particular time points, at the end of the packing, at the end of the cooling, and at $t=110$ [sec], at which time the part is almost cooled down to its storage temperature. It is clear that P is time and position-dependent, but not direction-dependent. More change of P happens in the centerline region due to the higher temperature there, and the less change occurs near the surface because of the lower temperature involved. Figure 4.3-16 is a plot of the gapwise profiles of the anisotropic stresses in the z -direction, σ'_{zz} , at the same time points as Figure 4.3-15. It is, of course, understandable that the anisotropic stresses σ'_{zz} must change with the time and position, because there is no total stress gradient in the z -direction throughout the part (Equation 4.31). The same reasoning having to do with temperature histories, can also explain that the anisotropic stresses change differently in the center and near the surface.

The total stress in the x -direction is defined by Equation 4.22. Figure 4.3-17 is a plot of the gapwise profiles of the total stresses in the x -direction, σ_{xx} , also at the same time points as Figure 4.3-15. It is assumed that $\sigma_{xx} = \sigma_{yy}$. It shows that the total stresses in the x -direction change with time and have gradients in the z -direction. It is noted that the profiles have similar shapes comparing with the literature data (Figure 4.3-11), but the total stresses change their signs from negative to positive. The total stresses in the x -direction are compressive in the early time and tensile later. This is because the whole part tends to cool down and to shrink faster, but the isotropic stresses inside the part prevent it. Then the part is subjected to compressive stresses in the x -direction. Later, as shown in Figure 4.3-15, the temperature has decreased so much that

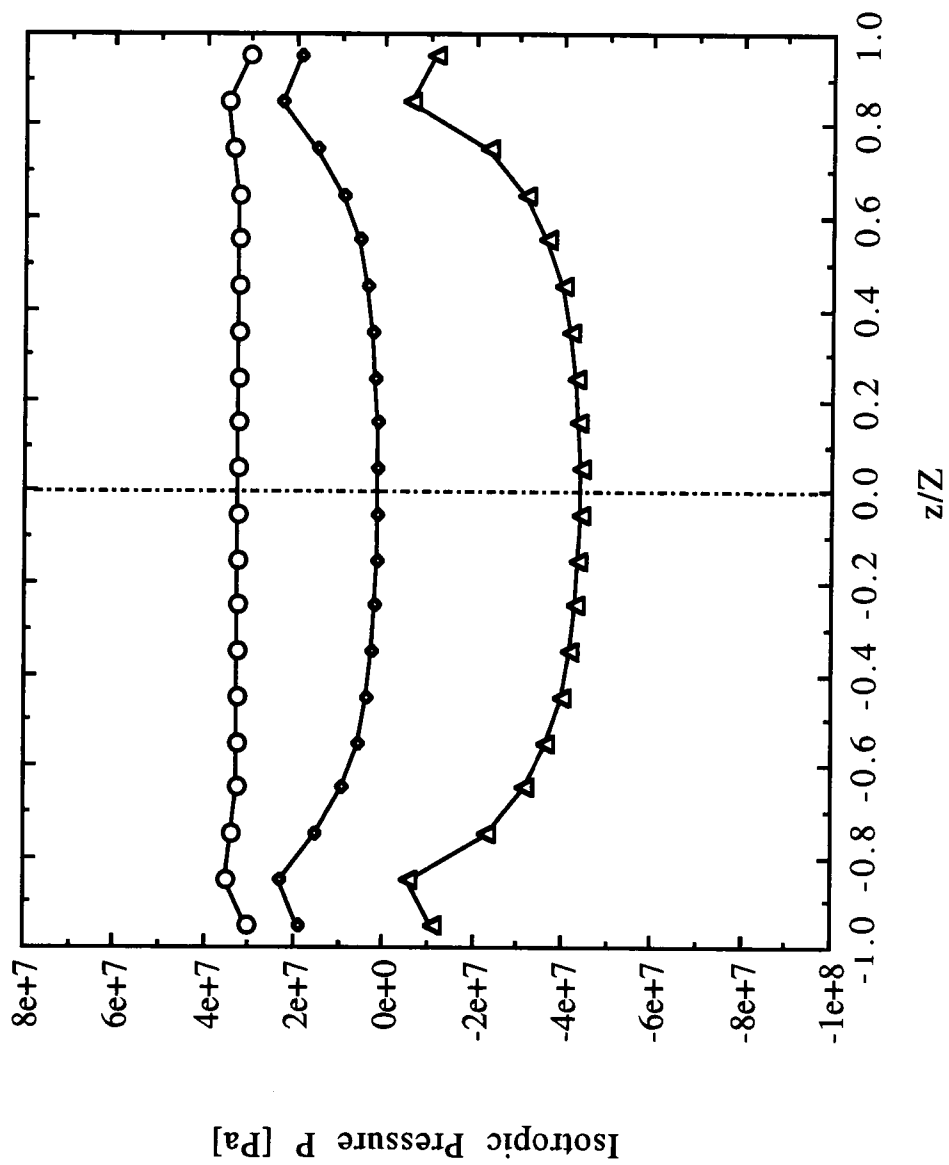


Figure 4.3-15 Predicted isotropic pressure profiles for Case II;
 —○— at 4 seconds; —◇— at 15 seconds; —△— at 110 seconds

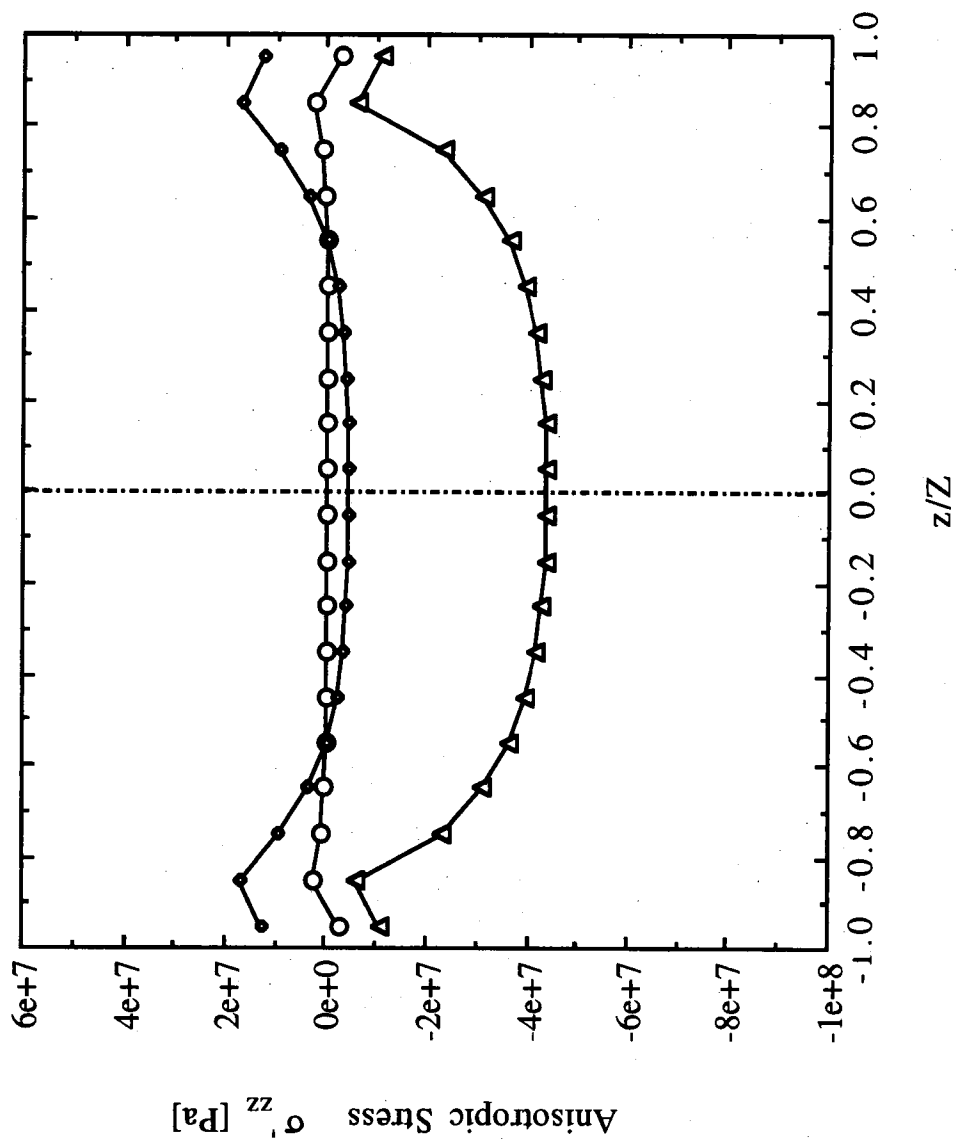


Figure 4.3-16 Predicted anisotropic stress profiles for Case II;
 —○— at 4 seconds; —◇— at 15 seconds; —△— at 110 seconds

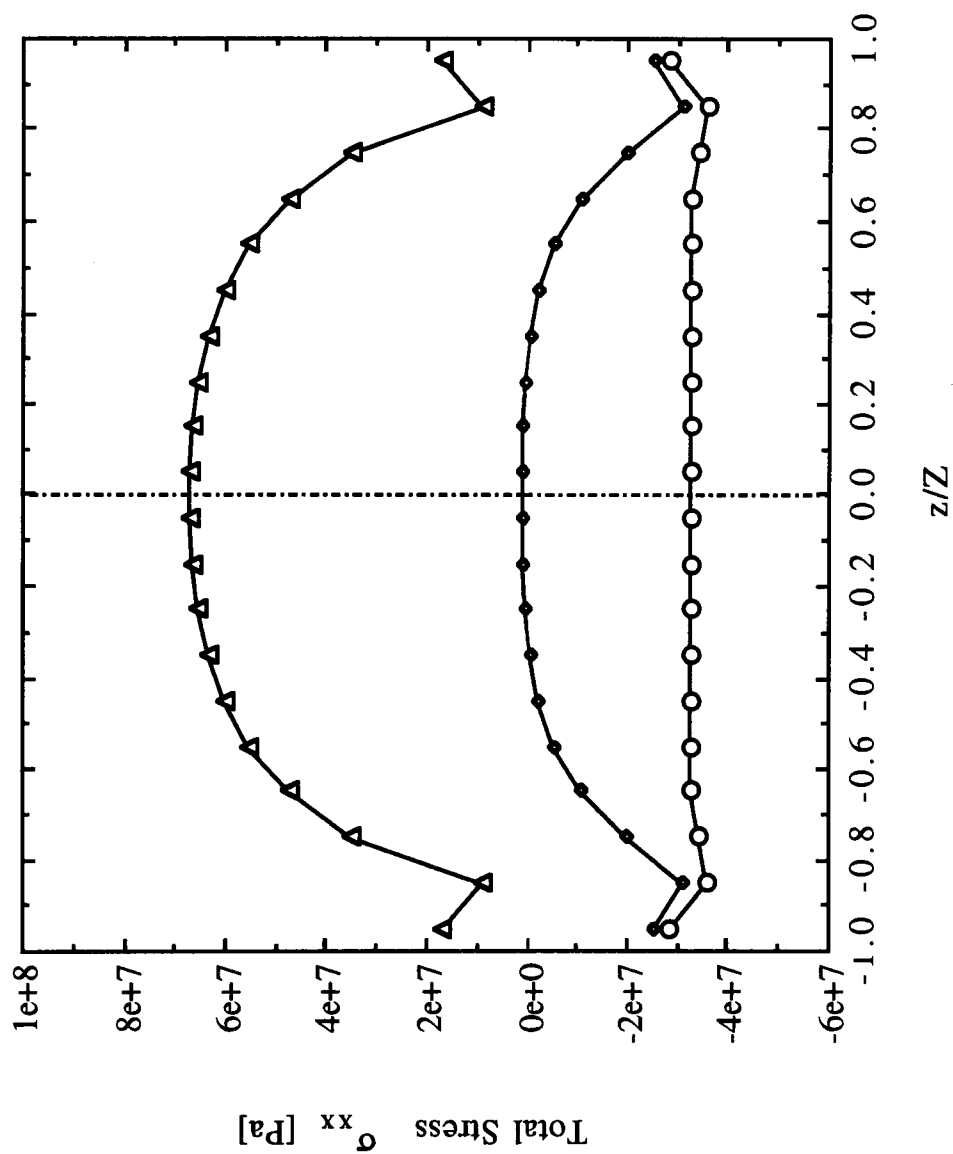


Figure 4.3-17 Predicted total stress σ_{xx} profiles for Case II;
 —○— at 4 [sec]; —◇— at 15 [sec]; —△— at 110 [sec]

the P becomes negative. Thus tensile stresses in the x -direction are introduced.

The predictions of the total stresses in the x -direction are not in agreement with the literature data, except that the shapes are similar. A comparison of the anisotropic component of the stresses with the data will be made to see whether there is any relationship between them. Figure 4.3-18 is a plot of the anisotropic stresses in the x -direction, σ'_{xx} ($= \sigma'_{yy}$) and the data of the Delft group (Figure 4.3-11), plotted here as a reference. The shapes of the anisotropic stresses in the x -direction are also similar with that of the literature data. It needs to be understood, however, the stresses that are measured came from slices that had been moved from the samples, but here the predicted stresses are those in the undisturbed state. Later an alternate way to simulate residual stresses will be presented which is probably closer to what is done experimentally.

The data (Figure 4.3-11) and the simulations (Figures 4.3-15, 4.3-16, 4.3-17 and 4.3-18) show sharp changes of the stresses near the surface. These sharp changes may be explained as follows. The surface layer is cooling at a higher rates and reaching a lower temperature at a very early stage; the packing pressure was applied under these conditions. The P in the surface layer is always lower than that in the second layer from the surface because of the higher cooling rates. Also the thermal histories result in more non-equilibrium density there; therefore, there is more anisotropic stress there. The total stress in the surface layer, determined by these two components, is higher than that in the second layer from the surface. In contrast, the layers near the center line are packed at a higher temperature and cooled at a lower rate. They have less non-equilibrium density frozen-in, but have a great amount of temperature cooling yet to be done. The large amount of the thermal shrinkage in these layers results in a lot of isotropic stress decrease and a great amount of anisotropic stress builds up. The combination effects of pressure, temperature, cooling rate and

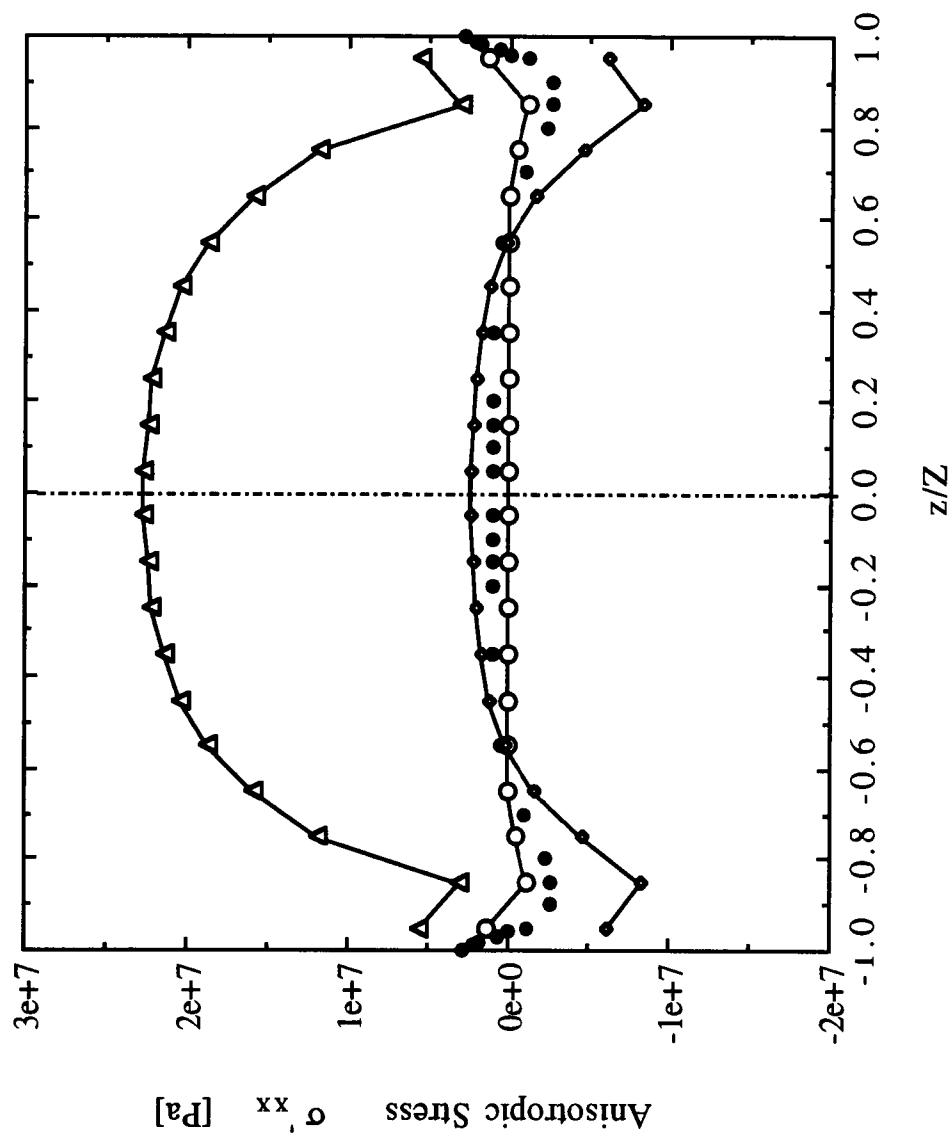


Figure 4.3-18 Predicted anisotropic stress σ'_{xx} profiles for Case II;
 • data of Delft;—○— 4 [sec]; —◇— 15 [sec]; —△— 110 [sec]

density change will attribute to the typical residual stresses distribution. But, it is not easy to separate these effects in practice. Thus, the present formulation (a PVT-time approach) is needed.

At the present time, these are very few residual stress data available. The few available data were measured from the post-ejection parts by special techniques such as the layer-removal method. That means the parts had to be cut into pieces to perform the measurements. Data for the actual stresses inside the whole part would be desirable, but are probably unattainable. The present framework is able to predict residual stresses inside the whole part during all three steps. However, the comparison here shows that differences between the simulation and the residual stress data from the literature are large. An alternate simulation, to be presented later, will attempt to deal with the conditions under which the experimental data were obtained.

§4.3.4.3 Pressure Decrease and Density Changes: Comparison of Simulation with Case III

Since the available data for Case III are of pressure and density distribution only, the discussion of the simulation here mainly focuses on these two subjects.

The predicted total pressure in the z-direction for Case III is presented in Figure 4.3-19. A notable difference between the data and the prediction at the time of $t \approx 8$ [sec] is due to the simplified parameters involved. The pressure compressibility coefficients, κ_r , κ_g and κ_a , and the thermal expansion coefficients, α_r , α_g and α_a , are not only temperature-dependent, but also pressure-dependent. In the present work, however, constant values were used except that the values change when temperature passes through the glass transition point. These discontinuities are in all cases. But the initial packing pressure is higher in Case III (78 [MPa]); in Cases I and II

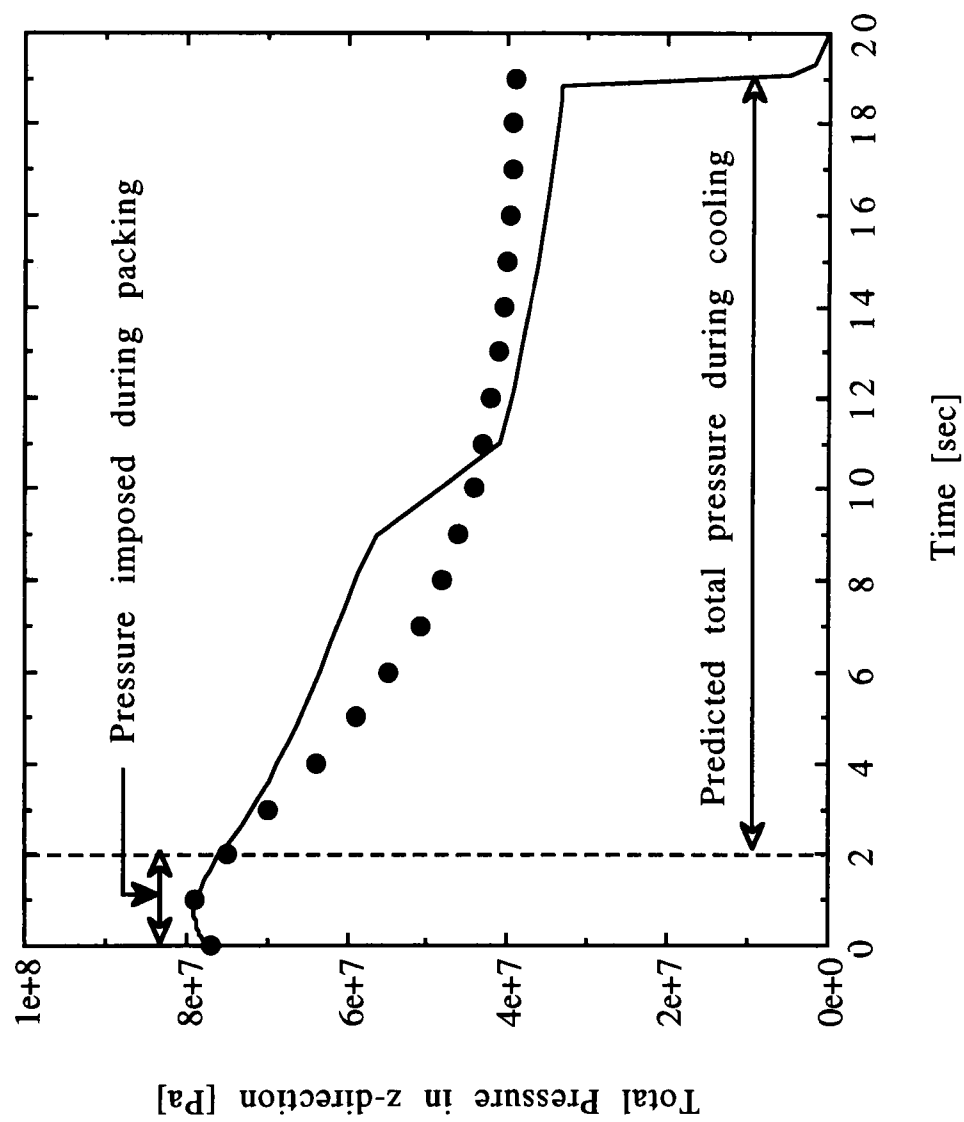


Figure 4.3-19 Comparison of the total pressure in the z-direction for Case III;
 — present work; • data of the Eindhoven group

the initial pressures are lower (47.4 and 42 [MPa], respectively). Therefore, in Case III, discontinuous change from κ_r to κ_g causes a big change in the specific volume. The predicted total pressure in the z-direction was affected by using the simplified parameters.

The predicted gapwise density distributions are plotted in Figure 4.3-20. Comparing this figure with 4.3-13, a qualitative agreement (similar shape) between the predicted density profiles and the literature density data was achieved, but the magnitudes are quite different. In the center area, there is a low plateau of density distribution which corresponds to the higher temperature and lower cooling rates there. A peak density is located below the surface which is related to the lower temperature and higher packing pressure there. It is found that the surface layers have a lower density than that in the second layer from the surface. That is because very high cooling rates and very low temperatures are involved there, and because the packing pressure is applied at the temperature lower than T_g .

It is noted that the density data from the literature were measured by cutting the specimens out of the molded part and putting them in a DGC. The data were taken after aging for two and nine days, respectively. These data are, therefore, not the actual density distribution inside the molded part. In other words, the data profiles (shape) may only remember some of the density distribution histories. Thus, the differences between the prediction and the data are perhaps understandable for the similar reasons as for the residual stress discussed in Case II.

The simulation also predicted all the components in terms of isotropic stress, anisotropic stress and total stress in the x and y-directions at various times and positions for Case III. Because there is the lack of the experimental data, only a cross comparison between Cases II and III was made. This will be done in the next section.

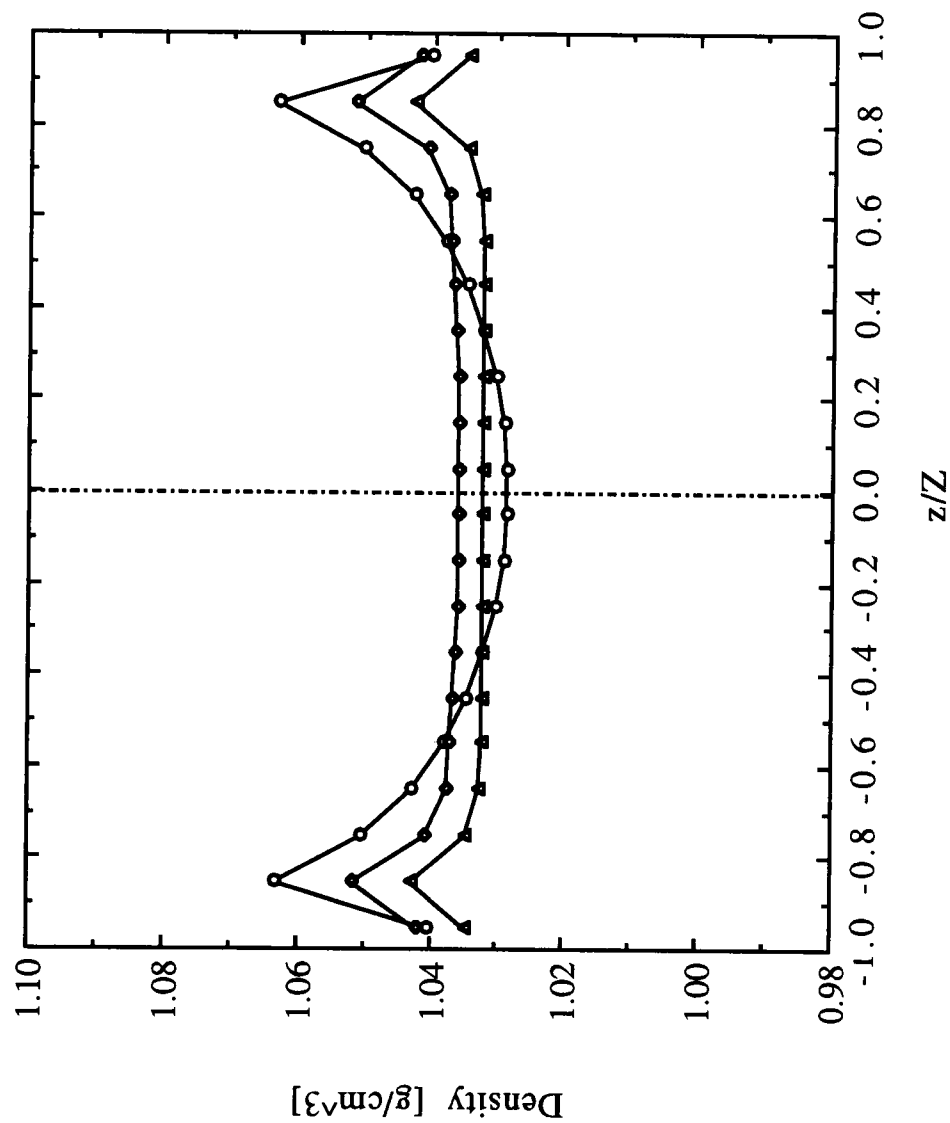


Figure 4.3-20 Predicted density profiles for Case III;
 —○— at 2 seconds; —◇— at 19 seconds; —△— at 110 seconds

§4.3.4.4 Comparison of the Simulations of the Two Cases Involving Different Injection and Post-ejection Histories

This section emphasizes results for Cases II (Delft) and III (Eindhoven) because data for the post-ejection step are available. Case I (Cornell) is not included but the conditions for the packing and cooling steps are very similar to those of Case II. As summarized in Table 4.3-1, the essential differences are the initial packing pressure=42 [MPa] and the storage temperature=-18 °C for Case II and the initial packing pressure=78 [MPa] and the storage temperature=23 °C for Case III. A comparison of the two simulations is made to see the relationship between the processing conditions and the residual stresses.

In this framework, the total stress σ_{zz} is composed of two components, an isotropic stress $-P$ and an anisotropic stress σ'_{zz} . The meaning of the terms of the isotropic pressure P here is in the sense of PVT relationship. It can be either sign. A positive P means it tends to reduce the volume, and a negative one tends to increase the volume. An important consequence of the framework is that while the total stress, σ_{zz} , does not vary with z , its isotropic and anisotropic components ($-P$ and σ'_{zz}) do. That means there are gradients of both P (thus $-P$ and σ'_{zz}) and temperature T in the z -direction. The total stresses in the x -direction are z -dependent because of the temperature gradients in the z -direction. The signs of the stresses are changed in accordance with the signs of the isotropic pressure P . A positive P introduces compressive total stresses in the x -direction and a negative P results in tensile total stresses.

Figure 4.3-21 is a plot of the predicted total stress profiles in the x -direction. From this figure, one notes that the predicted total stress profiles, σ_{xx} , are of similar shape to the data of the Delft group (Figure 4.3-11). The important facts here are that Case II has a

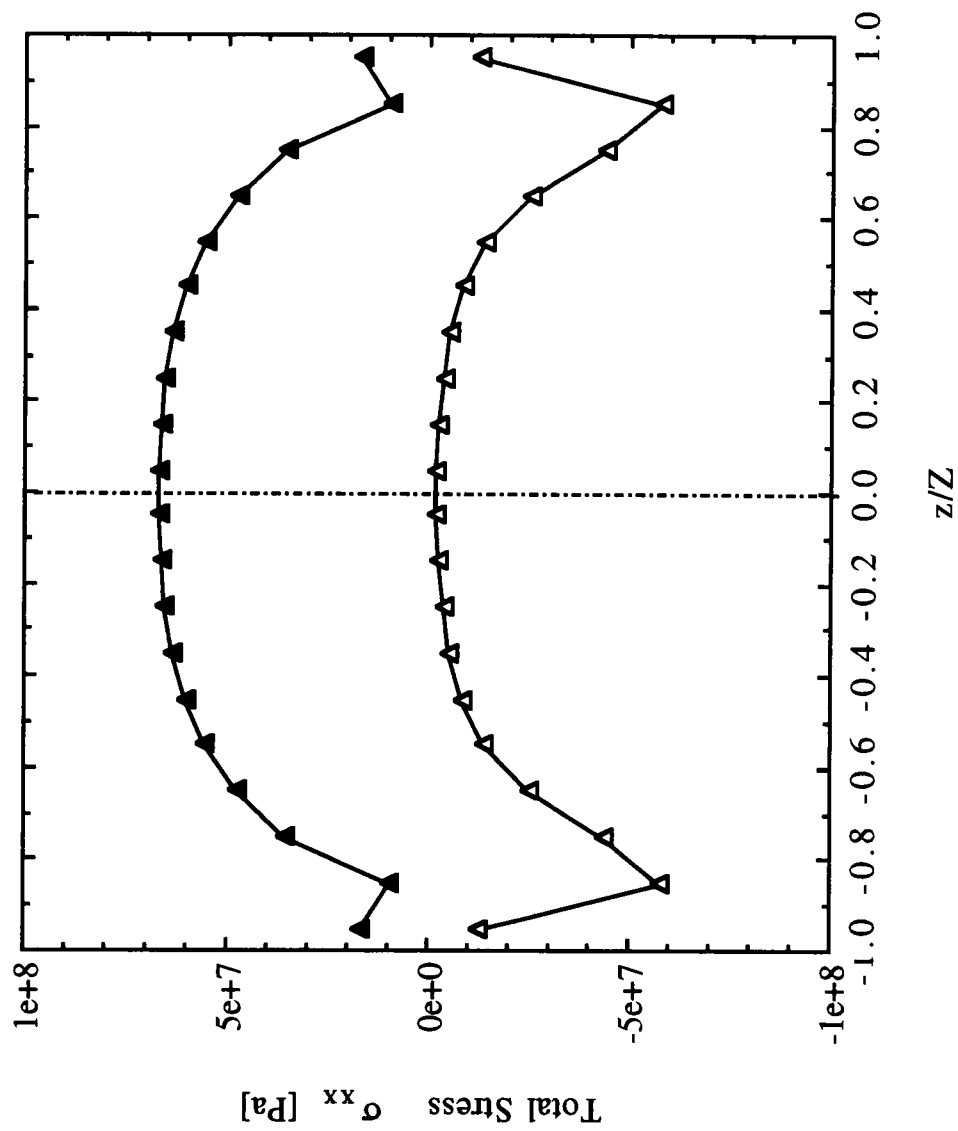


Figure 4.3-21 Predicted profiles of total stress σ_{xx} at $t=110$ seconds, —▲— Case II; —△— Case III.

tensile stress and Case III compressive stress. This is because of the different packing pressure and storage temperature involved. The higher packing pressure and storage temperature (Case III) result a positive P . In contrast, the lower packing pressure and storage temperature (Case II) result a negative P . These isotropic pressure at $t=110$ seconds are shown in Figure 4.3-22. The total stress is determined by Equation 4.22. Now, the whole part is already solid. A compressive total stress in Case III will physically maintain the part in stable. So does a tensile total stress in Case II. Figure 4.3-23 is a plot of the anisotropic stress profiles in the x -direction at $t=110$ seconds. It shows clearly that the anisotropic stress components correspond to the processing and post-ejection conditions. If Case II had not been cooled to $-18\text{ }^{\circ}\text{C}$, perhaps the P value would have remained. Figure 4.3-15 shows that P passes from positive to negative as time passes.

Figure 4.3-24 is a plot of the predicted density distributions at $t=110$ seconds. The predicted density profiles for Case III (Figure 4.3-20) have similar shapes as that of the literature data (Figure 4.3-13). But the magnitudes are very different; the data are in the range from 1.045 to 1.047 $[\text{g}/\text{cm}^3]$ and the prediction of Case III are in the range from 1.035 to 1.065 $[\text{g}/\text{cm}^3]$. Since no data are available for Case II, it can only be said that different processing and post-ejection conditions may result in different density distributions.

As mentioned before, there is the difference between the prediction of σ'_{xx} and the literature data. It would be encouraging to simulate the situation in a way which will make the simulation closer to the experimental conditions. This alternate simulation will now be reported.

§4.3.5 An Alternate Simulation of the Post-ejection Step

At the present time, there is the lack of experimental data for

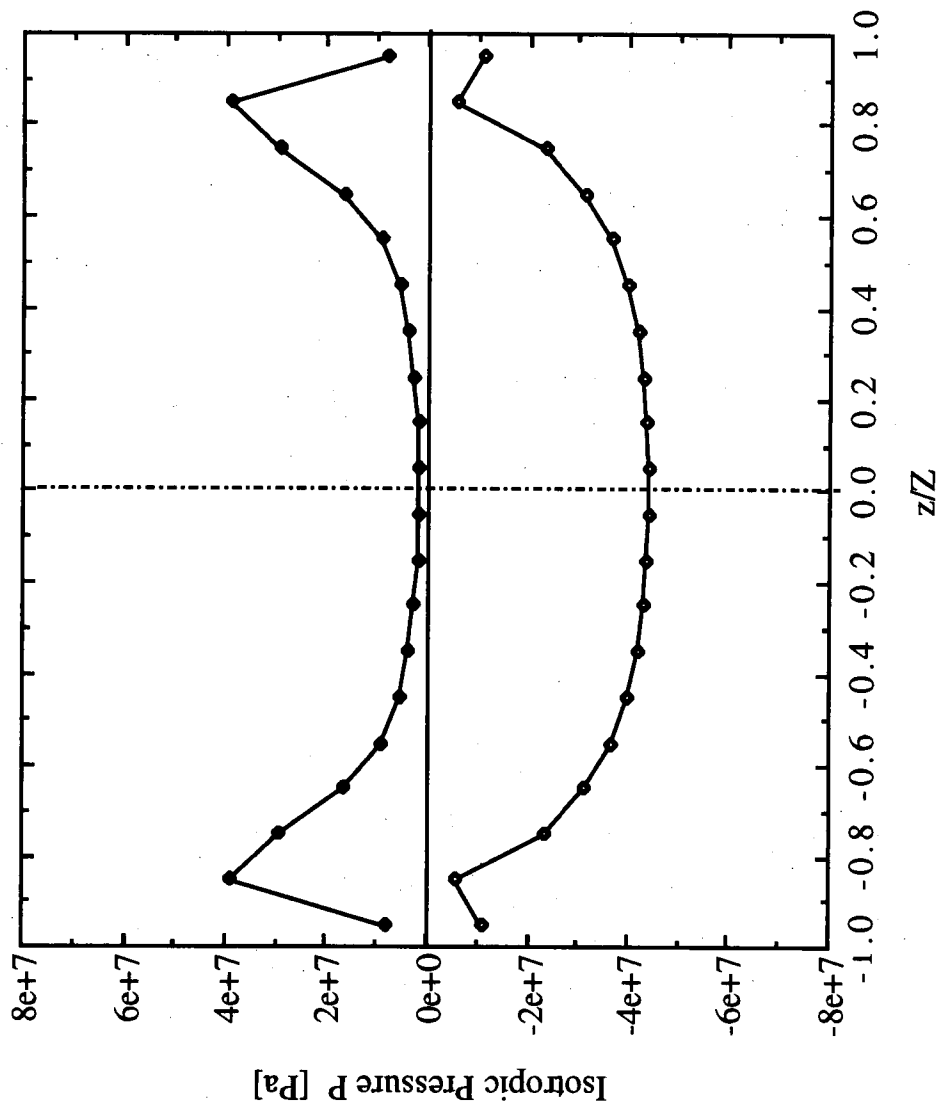


Figure 4.3-22 Isotropic pressure profiles at $t = 110$ seconds predicted by non-equilibrium formulation, $-\diamond-$ Case II; $-\bullet-$ Case III.

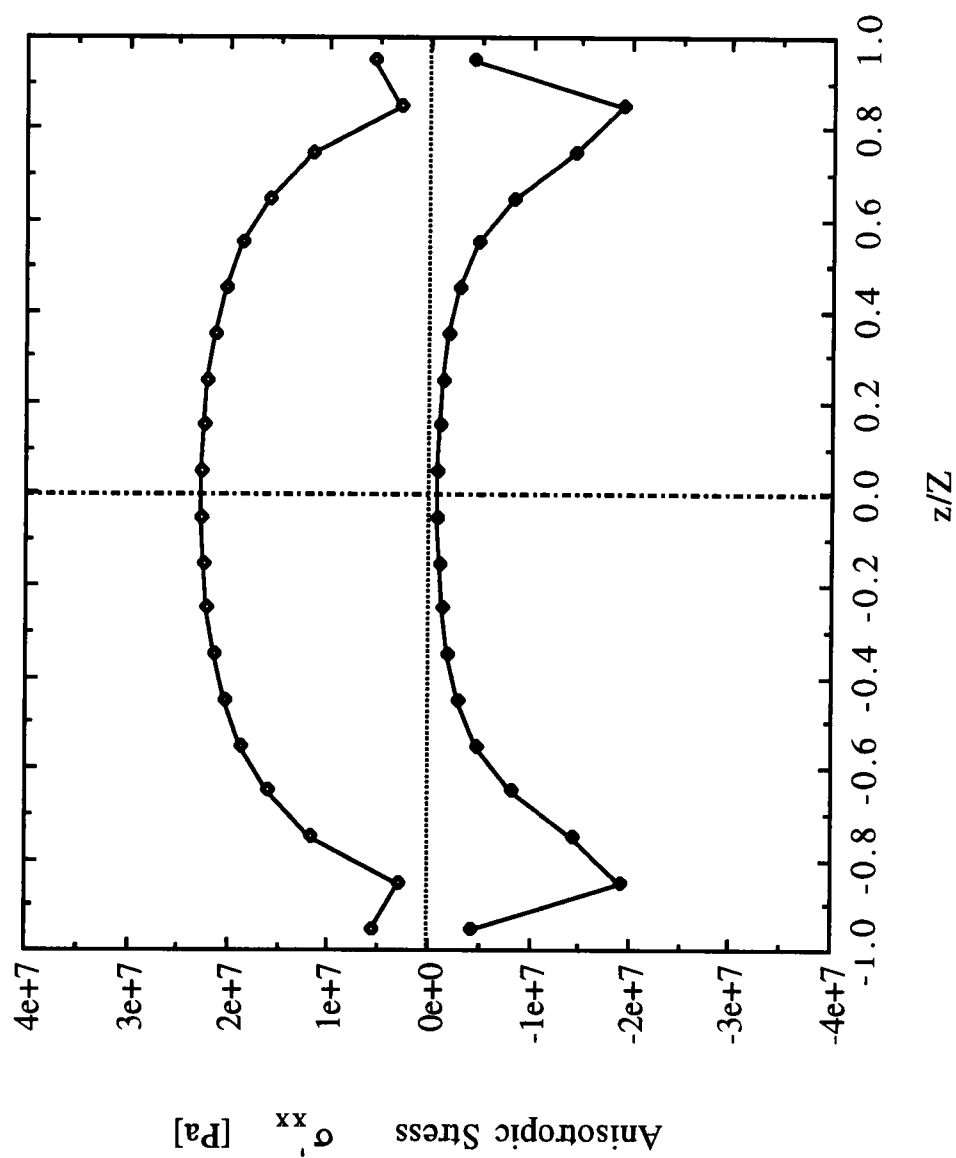


Figure 4.3-23 Predicted anisotropic stress σ'_{xx} profiles at $t = 110$ [sec], $\diamond$ — Case II; $\blacklozenge$ — Case III.

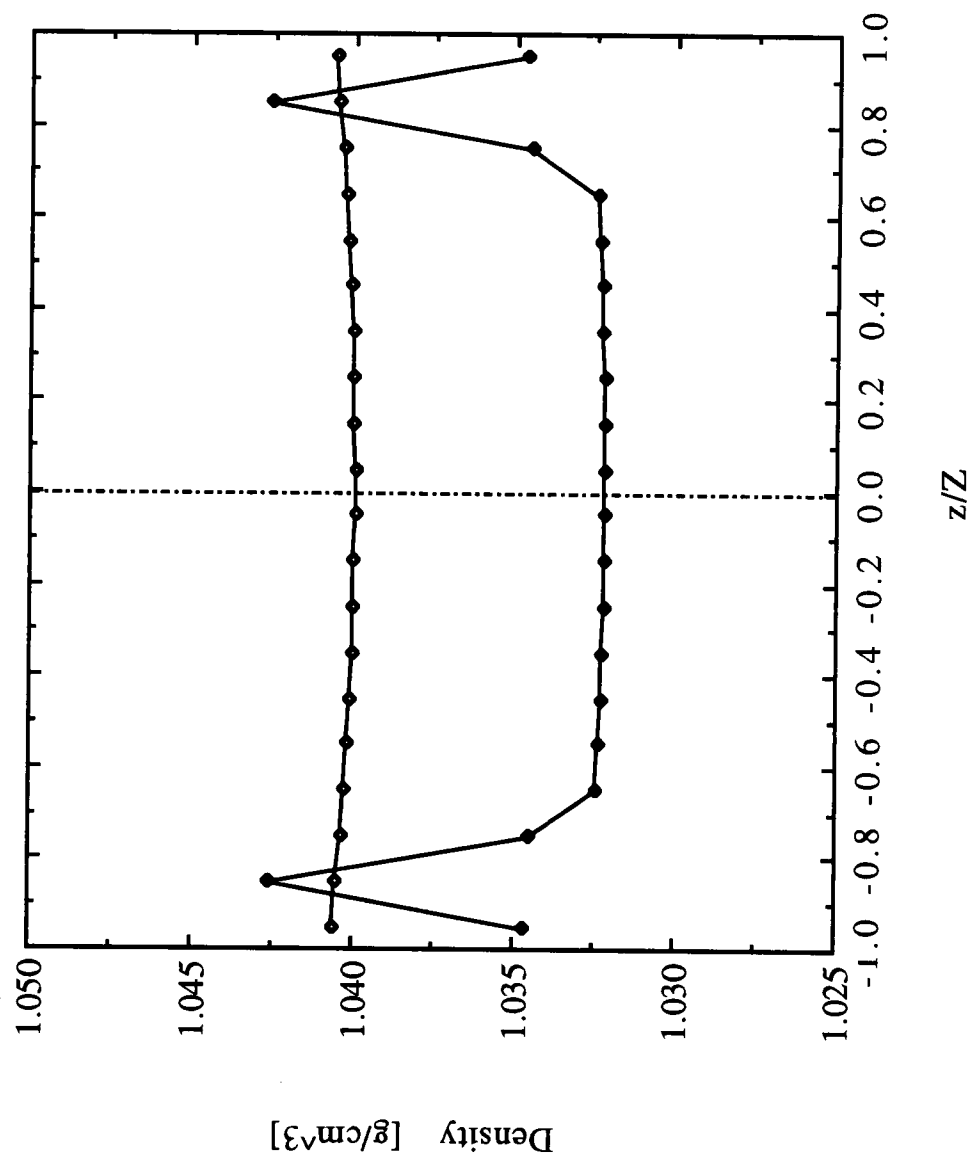


Figure 4.3-24 Predicted density profiles at $t = 110$ seconds,
 —◇— Case II; —●— Case III.

residual stresses which are obtained by a nondestructive method. It is desired to simulate an actual case including the processing, post-ejection and measuring procedures to pursue a better prediction for the residual stresses. For this purpose, an alternate analysis was done in terms of an alternate constraint. Two simulations, for Cases II and III, were carried out. there will be reported here.

The alternate simulations are based on the same formulation of the present work. Only one of the constraints used in the simulation of the post-ejection step was altered. Instead of Equation 4.35, the alternate constraint reads as

$$\sum_{i=1}^N \sigma'_{xx}(i,t) = 0 \quad (4.67)$$

This equation is formed by imagining that the post-ejection part has equally divided layers in the x-y plane. Similar as the free quench problem (classic residual stress problem), it is assumed that the ends of the long directions solidify as a "moving cage". That means that the long dimensions are required to contract uniformly. One can imagine that the layers of the part are more movable in the z-direction and connected mainly at the solidified ends in the x- and y-directions after the mold is opened. Now, when one does the layer removal, the constraints at the ends of the long directions are released. The isotropic stress may act to change the density (specific volume) but has nothing to do with the bending of the sliced layer. Then the anisotropic stresses cause the bending and are measured. Equation 4.67 describes this imagined picture. The constraint conditions used by the alternate analysis are summarized in Table 4.3-2. The results of the alternate simulation are discussed below.

Figure 4.25 is a plot of the total pressure profiles in the z-direction predicted by the alternate model. There is a numerical difficulty at the mold opens because one does not know the total

pressure at the end of cooling. Therefore, a slight discontinuity occurs in each pressure curve at that time point in Figure 4.3-25. It is noted that the total pressure in the z-direction is not zero after the mold opened. This result suggests that the solid portion of the part in which the temperature of the layers is lower than the glass transition temperature may retain some residual stresses after the mold is opened. Figure 4.3-26 is a plot of the total stress profiles in the x-direction at the end of the cooling step. Both cases are subjected to the compressive residual stress at this time. This is because the total physical part plays a role is holding a positive P inside the part, as presented in Figure 4.3-27. The predictions of the anisotropic stresses by the alternate model agree with the data of the Delft group which is shown by Figure 4.3-28. The results also indicates that the different conditions finally result in less effect on the anisotropic stress profile. The alternate simulations are not, however, able to predict density profiles that are in very good agreement with the literature data. The predicted density profiles are shown in Figure 4.3-29. It shows a reasonable distribution of the density except that there is the highest density in the surface layers. As shown in Figure 4.3-25, the total pressures are not zero after the mold is opened. This remained total pressure may increase the surface layers' density. It is noted that the available density data were measured by the DGC with the specimens cut from the parts. There are many time lags because of experimental difficulties. The predicted density profiles are of the density inside the parts. Thus, the essential difference in the density between the data and the simulations must be understandable.

Table 4.3-2
Summary of constraints used in the
basic and alternate simulations of post-ejection step

Type	Constraints	Equation	Notes
Basic Simulation	• constant total mass	$\sum_{i=1}^N m_i = M$	The total mass remains constant, the same as that at the end of packing, but the total volume varies. The applied pressure throughout the part is atmospheric.
	• zero applied pressure	$-\sigma_{zz}(i, t) = 0$	
Alternate Simulation	• constant total mass	$\sum_{i=1}^N m_i = M$	The total mass remains constant, the same as that at the end of packing, but the total volume varies. The applied pressure at the surface of the part is atmospheric, but it is not necessarily atmospheric throughout the part. The summation of the anisotropic stress in the x-direction over the thickness is zero.
	• zero applied pressure at the surface	$-\sigma_{zz}(N, t) = 0$ $\Delta\sigma_{zz}(i, t) = 0$ $i=1 \text{ to } N-1$	
	• zero summed edge stress	$\sum_{i=1}^N \sigma'_{xx}(i, t) = 0$	

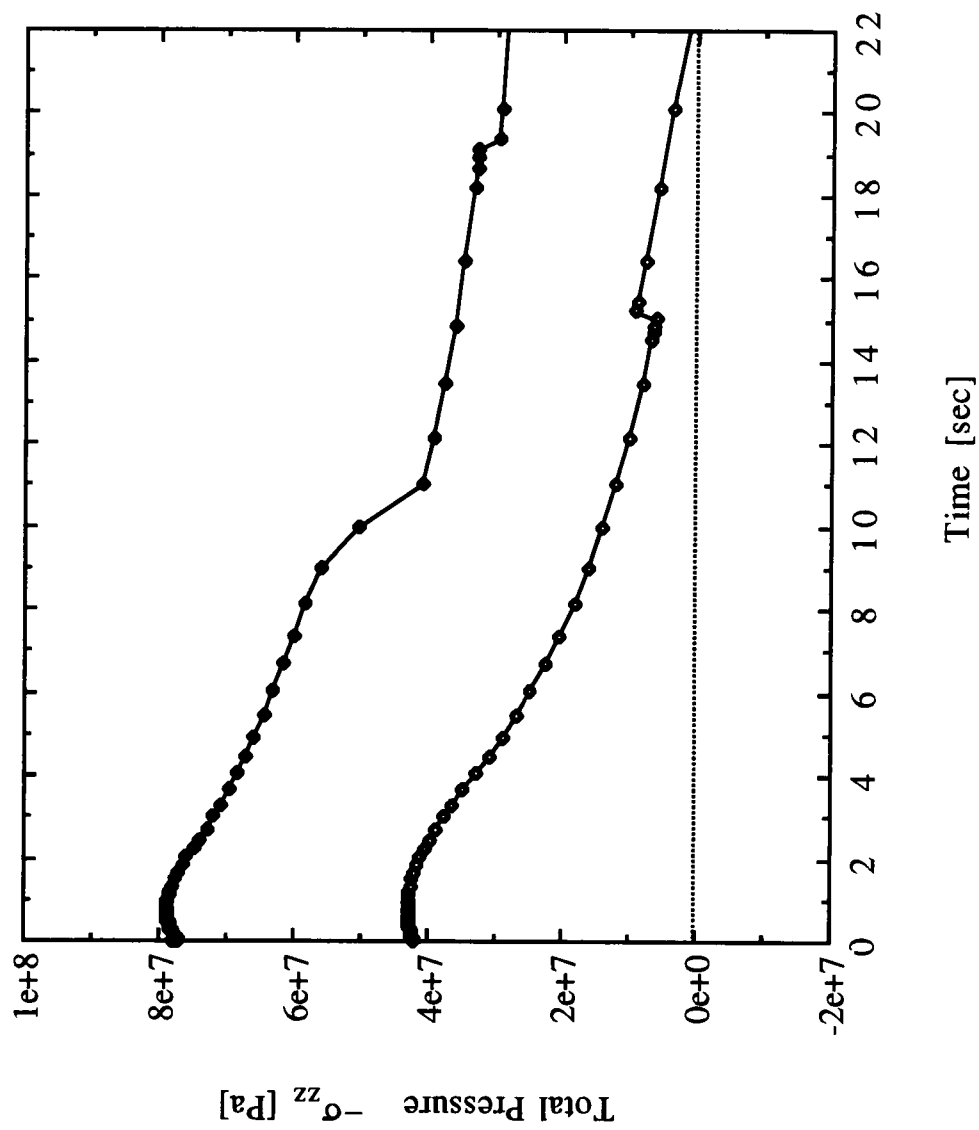


Figure 4.3-25 Total pressure profiles predicted by the alternate simulations; $\diamond$ —Case II; $\blacklozenge$ —Case III.

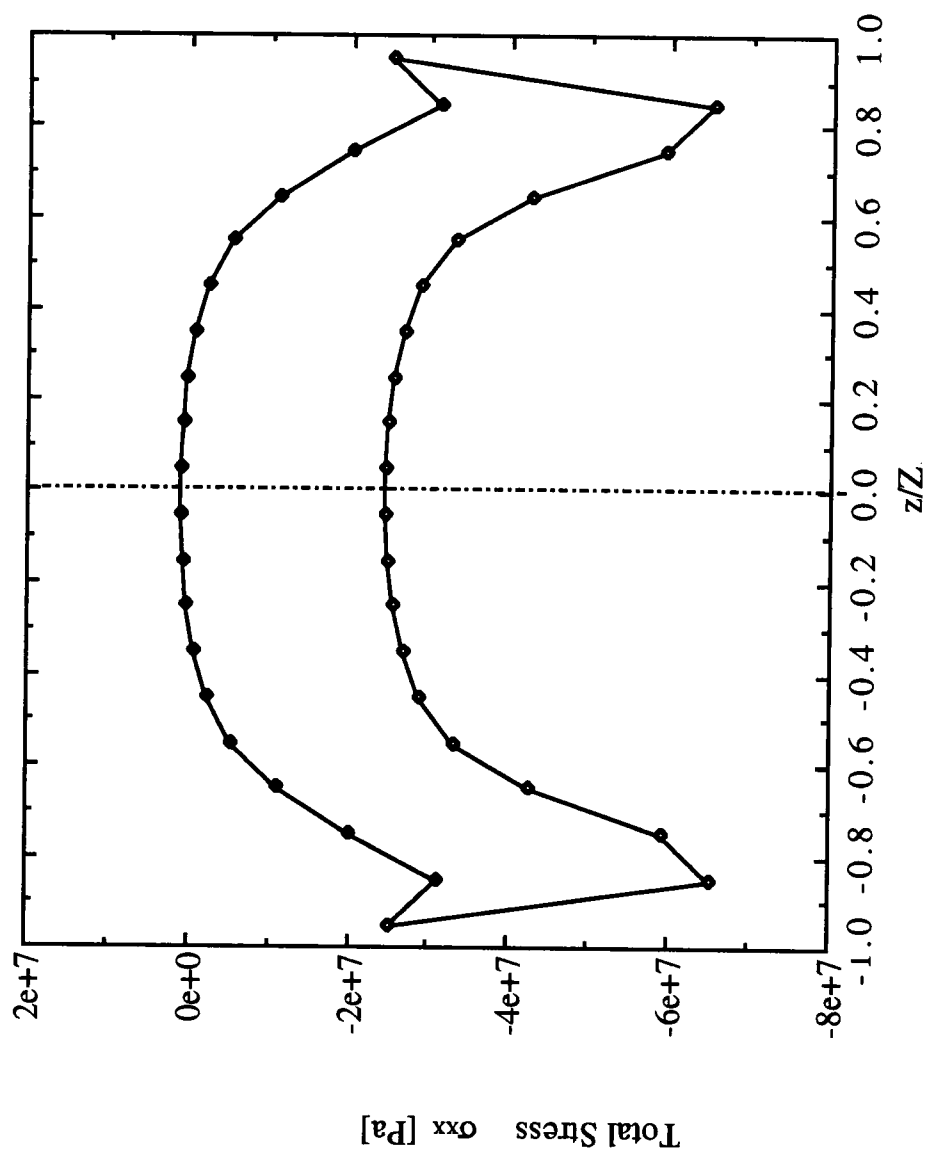


Figure 4.3-26 Total stress σ_{xx} profiles at the end of the cooling predicted by the alternate simulations; —♦— Case II; —◇— Case III.

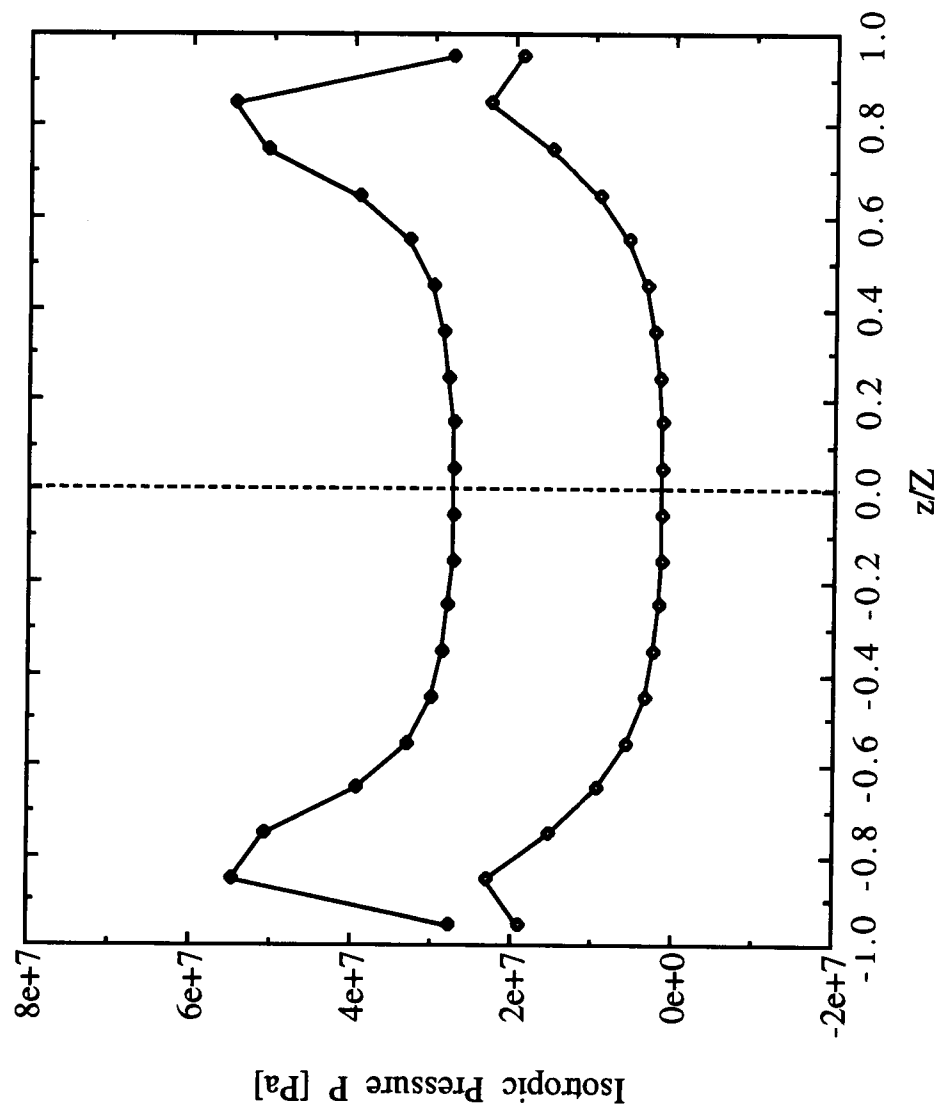


Figure 4.3-27 Isotropic pressure profiles at the end of cooling predicted by the alternate simulations; —○— Case II; —◆— Case III.

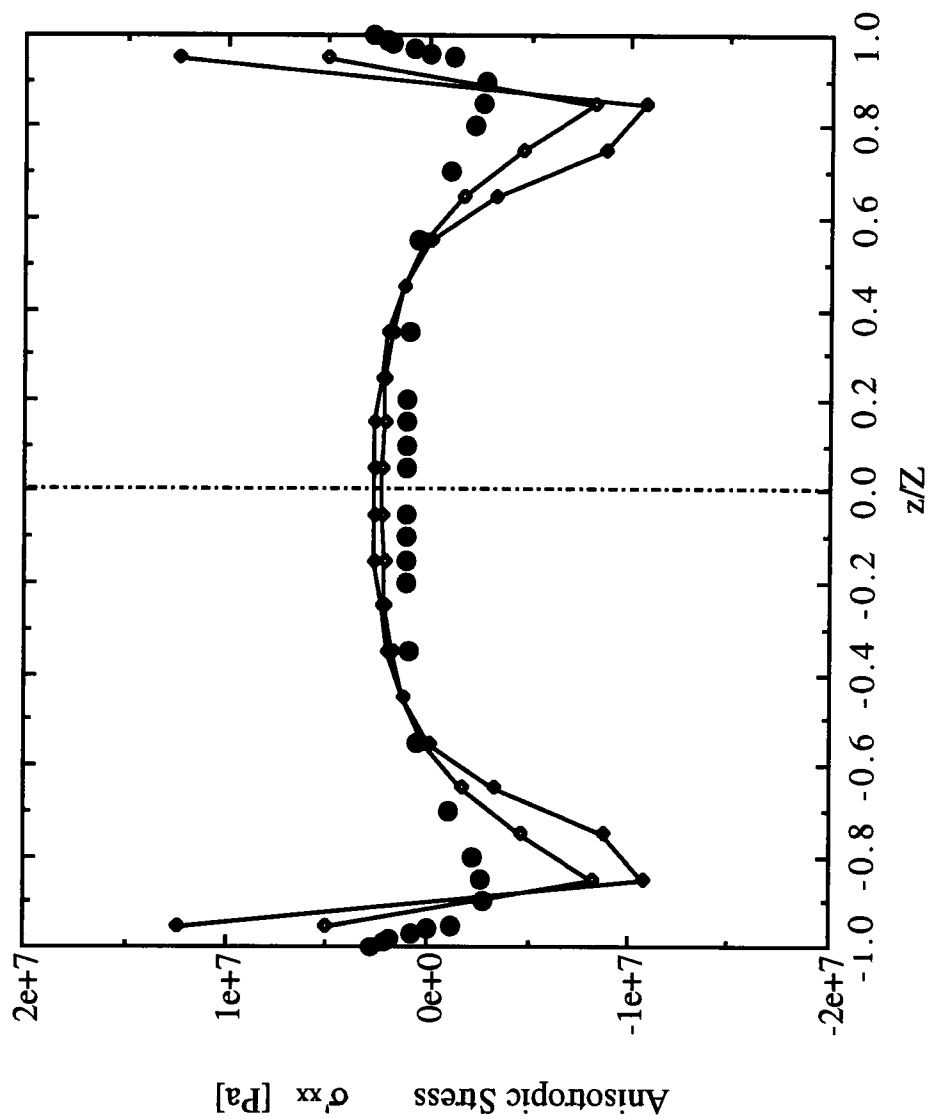


Figure 4.3-28 Anisotropic stress σ'_{xx} profiles at $t = 240$ [sec] predicted by the alternate simulations;
 —◇— Case II; —●— Case III; • data of the Delft group.

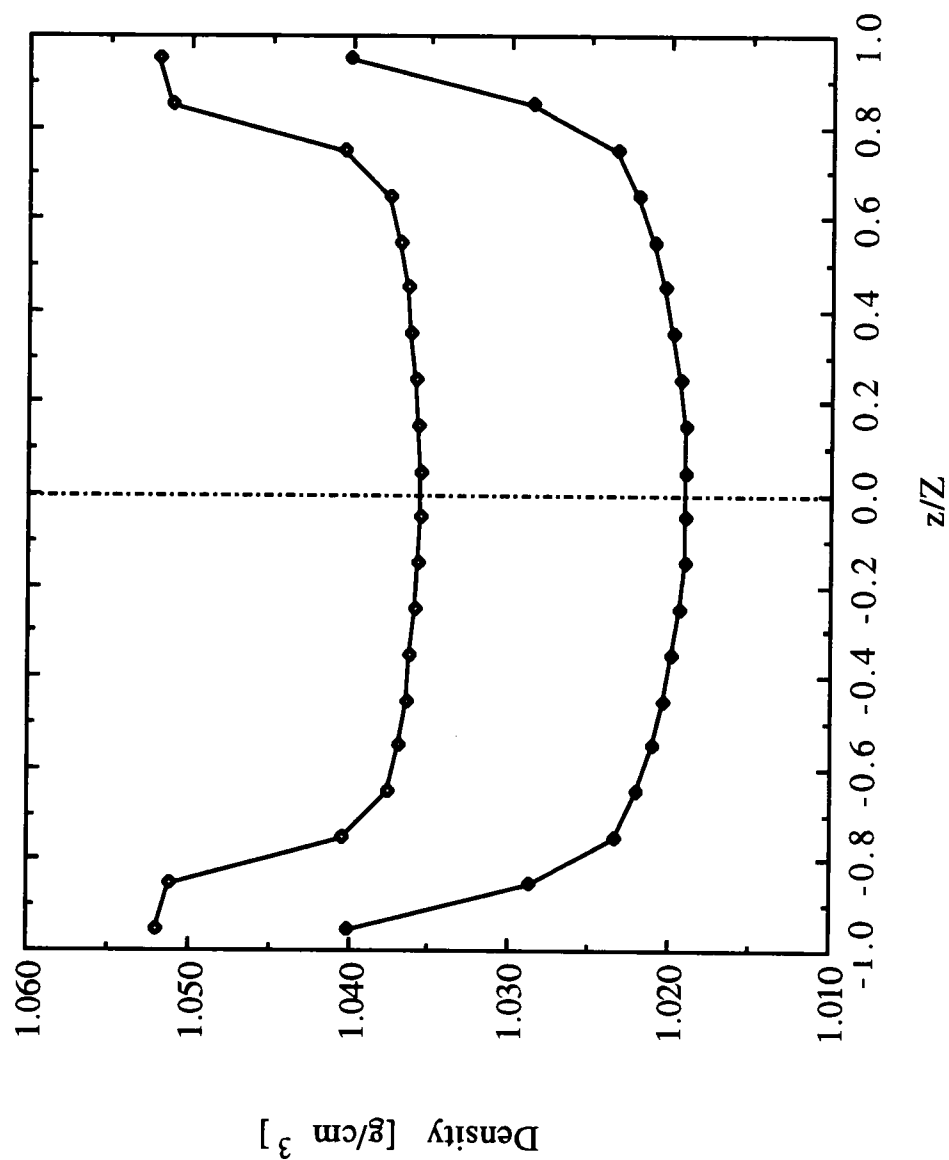


Figure 4.3-29 Predicted density profiles by the alternate simulations at $t = 110$ [sec]; —♦— Case II; —◇— Case III

CHAPTER 5

CONCLUSIONS

The present work is part of the continuing study of residual stresses and non-isothermal rheological behavior in polymer processing at the University of Tennessee. The present research consists of three parts: experiments and analysis of the time-dependent density changes in amorphous polymers; theoretical work on the development of time-dependent equations for the post-filling steps in injection molding; and use of these equations for simulating three experimental injection molding cases available in the literature. The major conclusions from this work will now be summarized.

§5.1. Time-dependent Density Changes in Amorphous Polymers

The experiments of this research involved measuring the cooling rates and the density changes by quenching bead-like of amorphous polystyrene with air and water. A special calibration procedure and analysis with hydrodynamic theory provided an estimate of the densities at the end of the quenches and the density changes during the subsequent aging. A rate equation was developed based on the present work. The time constant is related to the temperature, the cooling rate and the non-equilibrium density. Since it is difficult to separate these effects, a correlating variable and a rate-adjustable index were used to construct an empirical equation in which all the factors were included. Density changes at various cooling rates were predicted. These predictions are in agreement with the data of Greiner and Schwarzl and the data of the present work.

§5.2. Simulation of the Various Steps in Injection Molding

The injection molding process is complicated because it involves several steps (filling, packing, cooling and post-ejection). These steps are related to many parameters and processing conditions. In the present work a set of time-dependent equations to describe the density changes and residual stresses was developed. The theoretical work covered the post-filling steps in injection molding—that is, packing, cooling and post-ejection. A simple geometry (a rectangular slab with one thin dimension and two long dimensions) was used in this study. It is assumed that it is homogeneous in the x-y plane but with temperature gradients in the z-direction. This is only an approximation of the actual injection molding, in which there are gradients in the flow direction as well. The simulation consists of a set of simultaneous equations: a continuity equation, a force balance equation, an energy equation, a time-dependent PVT equation and a constitutive equation for the stresses. These equations must be solved simultaneously.

The energy equation reduces to classical transient heat transfer theory for a slab. An infinite heat transfer coefficient was used for the packing and the cooling steps and a finite heat transfer coefficient for the post-ejection step. The heat transfer equation was solved separately to obtain the temperature distribution in the slab. The simulation started with this z-dependent temperature distribution and an imposed time-dependent pressure distribution, simulating the end of the filling step.

The residual stresses introduced by the density changes were analyzed within the remaining simultaneous equations. The generalized anisotropic stress equations were reduced to two, $\sigma'_{xx}(=\sigma'_{yy})$ and σ'_{zz} . A new concept in the theoretical framework has to do with a kind of pressure P (an isotropic stress $-P$) that is used in the PVT equation—not, however, pressure in the ordinary sense. This “pressure” was introduced by Ko and Bogue to generalize the

framework of existing constitutive theory. Temperature and hydrostatic pressure necessarily affect the volume; but certain normal loadings (for example, tensile or compressive stresses) can affect it also. The generalized isotropic stress (-P) can be of either sign. This is very important in the constrained (residual stress) problem: through the thin dimension z , where the total stress σ_{zz} is a constant, there are gradients in both -P and the anisotropic stresses, often with a change of sign.

Allowing the anisotropic stress (σ'_{zz}) and isotropic stress (-P) to vary across z ($\frac{\partial \sigma'_{zz}}{\partial z} \neq 0$ and $\frac{\partial P}{\partial z} \neq 0$) even though the total stress gradient is zero ($\frac{\partial \sigma_{zz}}{\partial z} = 0$) is different from classical theory and is a physically important idea. Thus, for example, one can imagine a different P in each layer (as in Figure 4.3-22); the isotropic pressure is balanced by different anisotropic stresses in the various layers. This physical situation is not unlike that for a gas or liquid, for instance, trapped inside a metal tank—one can imagine a pressure gradient across the metal thickness, which causes anisotropic stresses there. By analogy one can imagine solid layers of polymer which trap hotter (soft) layers inside, the “pressure” of the trapped layers being of either sign, depending on the circumstances.

The most important term in the generalized PVT equation is the time constant $\tau(t)$. This empirical time constant is dependent upon the temperature, cooling rate, pressure and non-equilibrium density. It is shifted from a reference condition to a given conditions by those shift factors in which all factors are included in a correlating variable and a rate-dependent index.

The constraint conditions for the three steps in injection molding are different. During the packing step, the total volume of the part is that of the mold; and an imposed packing pressure is maintained by imagining that a small amount of material is added to

the cavity. In the cooling step, one presumes the volume and mass to be constant. While in the post-ejection step, the volume changes and the mass remains the constant, while also the applied pressure throughout the part is atmospheric.

The PVT-time equation and two stress equations are coupled in the formulation because density changes can induce stresses in a constrained sample and the stresses (deformations) can induce volume changes (the Poisson's ratio effect). Because this is a multiple variable problem subjected to the constraint conditions, a combination of calculation techniques with an optimum search method was employed in the simulations. The predictions are, finally, the "total stress" (pressure in the ordinary sense) as a function of time; and residual stresses and density distributions at various times.

§5.3. Comparison of Simulations with the Literature Data

Three cases with a similar geometry but different conditions were simulated by using the new framework. These cases approximated experimental data from groups at Cornell University, the Delft University of Technology and the Eindhoven University of Technology.

The PVT-time model of the present work was applied to simulate the total pressure versus time data for the packing and cooling steps of the Cornell group. The prediction was in good agreement. For comparison two equilibrium (not time-dependent) approaches were carried out with very small time constant. The first approach is based on the actual PVT data with $T_{ge}=87.2\text{ }^{\circ}\text{C}$. The second one is a T_g -shifted model of $T_{ge}=103\text{ }^{\circ}\text{C}$. Neither of these approaches yielded a satisfactory prediction, but the T_g -shifted model obviously improved the prediction. It is understood that the T_g -shifted model is an approximation of the non-equilibrium approach for a cooling rate of about $10\text{ }[^{\circ}\text{C}/\text{sec}]$. It was concluded

that the time-dependent density changes play an important role in the situation in which a high cooling rate involves, and that a time-dependent model is necessary for the simulation. A similar conclusion resulted from studies of total pressure versus time for the cases of the Delft and the Eindhoven groups.

The simulations of the Delft and Eindhoven cases covered all the post-filling steps, including post-ejection. (For the Cornell case the only data available was the decrease of pressure during cooling, as discussed in the previous paragraph.) The details of what happens inside the samples for these two cases are of interest because the packing pressures and storage temperatures are quite different: 42 [MPa] and -18 °C for the Delft case; 78 [MPa] and 23 °C for the Eindhoven case. Although the total stress (σ_{zz}) is constant in the z-direction, its isotropic ($-P$) and anisotropic (σ'_{zz}) components are not. Most of the time P is positive (that is, a compressive stress) and since the P term is larger than or equal to the σ'_{zz} and σ'_{xx} terms, the residual stresses are also compressive. But for the Delft case the combination of a lower packing pressure and low storage temperature results finally in a negative P (that is, a tensile stress) and consequently a larger specific volume. These unexpected results suggest that perhaps one needs to focus on the isotropic (P) component of the residual stresses (a kind of "trapped pressure", of either sign), rather than on the anisotropic component, as has been the case in classical residual stress theory. The influence of P on the physical properties may be a more significant factor than the gradient of anisotropic stresses ("compressive on the surface, tensile in the middle"), characteristic of classical theory.

Unfortunately, these predictions for residual stresses and densities cannot be tested directly because the present formulation predicts values for an undisturbed sample. In practice the sample must be cut up for testing, which releases part of the stresses. An alternate simulation was therefore performed, in an attempt to simulate what was done experimentally. It is assumed that only the

anisotropic stresses, not the isotropic stresses, can bend the sliced layers. The bending can be measured by the layer removal method. This alternate simulation predicted the measured residual stresses quite well in terms of both shape and magnitude, although perhaps fortuitously. Some features of the density distribution could be predicted qualitatively, although not quantitatively.

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APPENDICES

APPENDIX A

COMPUTER SIMULATION PROGRAM OF PACKING AND COOLING STEPS FOR THE CORNELL GROUP CASE

```
100 REM   Computer Simulation Program of Packing and Cooling
        Steps for the Cornell Group Case
111 REM   This Program Stops at t =16 [sec]

122 OPEN "CGCP.dat" FOR OUTPUT AS #1
124 OPEN "CGCY.dat" FOR OUTPUT AS #2
126 OPEN "CGCS.dat" FOR OUTPUT AS #3
128 OPEN "CGCV.dat" FOR OUTPUT AS #4
130 OPEN "CGCO.dat" FOR OUTPUT AS #5
132 OPEN "CGCG.dat" FOR OUTPUT AS #6
134 OPEN "CGCR.dat" FOR OUTPUT AS #7
136 OPEN "CGCT.dat" FOR OUTPUT AS #8
138 OPEN "CGCX.dat" FOR OUTPUT AS #9
140 OPEN "CGCD.dat" FOR OUTPUT AS #10
142 OPEN "CGCb.dat" FOR OUTPUT AS #11

145 REM M0 is the terms of summation of heat transfer equation
        before mold opens
150 REM Ma is the terms of summation of heat transfer equation
        after mold opens
152 REM U0 is the control of time increment
154 REM TI is the number of layers of half thickness
156 REM Hk is for  $h_{tc}/k$ 
158 REM NF is the number of simultaneous equations
160 REM AF is the thermal diffusivity
162 REM Ts is the starting temperature
164 REM Tw is the wall temperature
166 REM Tz is the initial temperature for post-ejection step
168 REM CN is the up limitation of iteration number
170 REM Kr0 is pressure compressibility coefficient of rubber state
172 REM Kg0 is pressure compressibility coefficient of glass state
174 REM Ka0 is the average pressure compressibility coefficient
176 REM P0 is the initial packing pressure
178 REM tp is the time point of the end of packing
180 REM tc is the time point of the end of cooling
182 REM NL is the limitation of data dimension
```

```

210 M0=60
215 Ma=26
225 U0=40
230 TI=10
235 Hk=4.762
240 Bb=-500
250 NF=3
270 AF=7*10^(-4)
275 Ts=200
280 Tw=32
285 Tz=75
300 CN=30
310 Kr0=9.3*10^(-10)
330 Ka0=7.3*10^(-10)
340 P0=4.74*10^7
350 Kg0=5.3*10^(-10)
360 tp=2
365 tc=16
370 NL=30

400 DIM N(TI),H(TI),TG(TI),FG(TI),GF(TI),iT(TI),Mv(TI)
410 DIM TT(TI),DT(TI),PP(NL),Q(CN,NL),PF(CN,NL)
420 DIM F(NL,NL),V(NL,NL),P(NL,NL),T(NL,NL),S(NL,NL)
430 DIM K(4,NL),FS(NL),DS(K0),TD(NL,K0),Tv(Ti),Tm(Ti)
440 DIM U(NL,Ti),W(NL),D1U(NL,NL),D1W(NL),EFA(NL),EFB(NL)
450 DIM Kr(NL),Kg(NL),Ar(NL),Ag(NL),TpS(NL),EFC(NL),EFD(NL)
460 DIM CC(K0,UK),NAR(NL),GRG(NL),DP(NL)
470 DIM PG(NL),GV(NL),VG(NL),DV(NL),Ka(NL)
480 DIM EV(NL),VE(NL),VR(NL),TA(NL),Aa(NL),Vv(NL)
490 DIM STR(NL),TAG(NL),TAU(NL),VY(NL),DVY(NL)

500 S0=10.65
510 S1=0.8
540 GOTO 8010
550 GOTO 7200
580 gosub 6500
620 FOR K=-5 TO 20 step 0.1
630 uu=int(U0/(abs(k)+2))
640 ED=(exp(k+0.1)-exp(k))/uu
645 D1=ED/2
650 U=1
652 FOR X=0 TO CN

```

```

653 FOR Y=0 TO NL
654 Q(X,Y)=0
655 PP(Y)=0
657 NEXT Y
658 NEXT X
663 S=s+ed
665 S1=S1+ed
667 S2=S2+ed
669 IF s>360 then 9910
670 FOR X=1 TO TI
680 GOSUB 2220
690 NEXT X
700 CC=0
710 cc=cc+1
715 if s > tc then 730
720 if S> tp then 750
730 Le=1
740 goto 760
750 Le=2
760 FOR L=TI TO Le STEP -1
770 GOSUB 1110
780 FOR Y1=1 TO TI
790 Q(CC-1,Y1)=Q(CC,Y1)
800 DV(Y1)=Q(CC,Y1)
810 NEXT Y1
815 NEXT L
816 IF s<=tc then 820
817 IF ABS(F0)<1*100 THEN 824
818 goto 822
820 IF ABS(F0)<1*10^5 THEN 824
822 IF CC<CN THEN 710
824 GOSUB 9710
826 GOSUB 2010
830 if s > (tc+0.5) then 875
835 if s < (tc-0.5) then 875
840 gosub 6500
875 U=U+1
880 IF U<=Uu THEN 652
885 gosub 6500
890 NEXT K
900 GOTO 9910

```

```

1100 REM Subprogram of Optimization and Multimodal Searching
1110 P1=-0.03
1125 P2=0.03
1220 P=P1
1230 GOSUB 3810
1240 F1=FSV
1260 P=P2
1270 GOSUB 3810
1280 F2=FSV
1290 P3=P2-OPT*(P2-P1)
1300 P=P3
1310 GOSUB 3810
1320 F3=FSV
1330 P4=P1+OPT*(P2-P1)
1340 P=P4
1350 GOSUB 3810
1360 F4=FSV
1400 IF ABS(P2-P1)<5*10(-6) THEN 1600
1410 IF F3>=F4 THEN 1500
1420 P2=P4
1425 F2=F4
1430 P4=P3
1440 P3=P2-OPT*(P2-P1)
1450 F4=F3
1460 P=P3
1470 GOSUB 3810
1480 F3=FSV
1490 GOTO 1400
1500 P1=P3
1505 F1=F3
1510 P3=P4
1520 F3=F4
1530 GOTO 1330
1600 IF F3<=F4 THEN 1630
1610 PP(L)=P4
1615 F0=F4
1620 GOTO 1650
1630 PP(L)=P3
1640 F0=F3
1650 P=PP(L)
1655 GOSUB 3810
1660 RETURN

```

2000 REM Subprogram for storing iteration data

```
2010 FOR X=TI TO 1 STEP -1
2011 U(X,0)=U(0,X)
2012 U(0,X)=W(X)
2014 D1U(0,X)=D1W(X)
2030 P(X,0)=V(X,1)
2033 PF(X,0)=F(X,1)
2036 S(X,0)=V(X,2)
2064 T(X,1)=TAU(X)
2066 T(X,2)=TAG(X)
2068 T(X,3)=NAR(X)
2070 T(X,4)=P(X,0)-S(X,0)
2072 T(X,5)=TT(X)
2074 T(X,6)=V(X,3)
2076 NEXT X
2100 if s > tc then 2155
2105 REM for packing and cooling steps
2110 tm=0
2112 for x=1 to Ti
2114 tm(x)=V0/U(0,x)
2116 tm=tm+2*tm(X)
2118 next x
2120 hx=hx0
2124 hy=hy0
2128 hz=h*2
2130 ad=tm/sv0/2
2133 tv=2*sv0
2134 tm0=tm
2140 tv0=tv
2145 goto 2190
2150 REM for post-ejection step
2155 Tv=0
2157 for x=1 to Ti
2160 Tv(X)=tm(X)*U(0,x)
2165 tv=tv+2*tv(X)
2170 next x
2172 tm=tm0
2174 xyz=1+(tv-tv0)/3/tv0
2176 hx=hx*xyz
2178 hy=hy*xyz
```

```

2180 hz=hz*xyz
2182 ad=tm0/tv
2184 tv0=tv
2186 tm0=tm
2190 RETURN

```

```

2200 REM Subprogram for temperature

```

```

2220 if TT(X) > Tw then 2260
2230 TT(X)=Tw
2240 goto 3350
2260 if s > tc then 9910
2350 Ss=s1
2370 Tw=32
2390 S2=0
2400 goto 3010
2420 REM Temperature for the post-ejection step
2440 Ss=s2+S0
2470 Tw=23
2540 T=0
2550 DT=0
2560 sm=1
2610 EFA(X)=0
2620 EFB(X)=0
2630 EFC(X)=0
2640 EFD(X)=0
2650 xa=(H-H(X))/(2*SQR(AF*Ss))
2660 xb=(H+H(X))/(2*SQR(AF*Ss))
2670 xc=hk*SQR(AF*Ss)+xa
2680 xd=hk*SQR(AF*Ss)+xb
2690 xe=hk*(H-H(X))+hk*hk*AF*Ss
2695 xf=hk*(H+H(X))+hk*hk*AF*Ss
2700 FOR m=0 TO Ma
2705 mm=1
2710 FOR mn=1 TO m
2720 mm=mm*mn
2730 NEXT mn
2740 EFA(X)=EFA(X)+(sm*(xa)^(2*m+1))/mm/(2*m+1)
2750 EFB(X)=EFB(X)+(sm*(xb)^(2*m+1))/mm/(2*m+1)
2760 EFC(X)=EFC(X)+(sm*(xc)^(2*m+1))/mm/(2*m+1)
2770 EFD(X)=EFD(X)+(sm*(xd)^(2*m+1))/mm/(2*m+1)
2780 sm=sm*(-1)

```

```

2790 NEXT m
2800 EFA(X)=1-2*EFA(X)/(SQR(IP))
2820 EFB(X)=1-2*EFB(X)/(SQR(IP))
2830 EFC(X)=1-2*EFC(X)/(SQR(IP))
2840 EFD(X)=1-2*EFD(X)/(SQR(IP))
2850 if TT(X)<=Tw then 2880
2860 Tm=1-EFA(X)-EFB(X)+EXP(xe)*EFC(X)+EXP(xf)*EFD(X)
2870 goto 2900
2880 Tm=0
2900 T=Tw+(Tz-Tw)*Tm
2940 IF T>Tz THEN 2980
2950 IF T>Tw THEN 2990
2960 T=Tw
2965 dt=0
2970 GOTO 2995
2980 T=Tz
2990 dT=(T-TT(X))/ed
2995 Goto 3135

3000 REM Temperature for the packing and cooling steps
3010 T=Tw
3020 DT=0
3030 SM=1
3040 FOR M=0 TO M0
3050 MPH=(M+.5)*IP/H
3060 Tm=2*(Ts-TW)*SM/MPH*COS(MPH*H(X))*EXP(-
    MPH*MPH*AF*Ss)/H
3070 T=T+TM
3080 DT=DT-MPH*MPH*AF*Tm
3090 Sm=Sm*(-1)
3100 NEXT M
3110 IF T>Ts THEN 3130
3115 IF T>Tw THEN 3135
3120 T=Tw
3125 GOTO 3135
3130 T=Ts
3135 TT(X)=T

```

3140 REM Subprogram for elastic modulus, parameters and
constants

3143 IF TT(X)>120 THEN 3180
3146 IF TT(X)<80 THEN 3190
3150 G1=0
3155 G2=0
3160 IF Tt(X)>100 THEN 3170
3164 G0=-97959+3244.8*tt(X)-34.9*tt(X)*tt(X)+.123*tt(X)*tt(X)*tt(X)
3166 G0=G0*10^6
3168 GOTO 3195
3170 G0=10^(652-17*tt(X)+.149*tt(X)*tt(X)-.00044*tt(X)*tt(X)*tt(X))
3175 GOTO 3195
3180 G1=0
3183 G2=1
3186 GOTO 3195
3190 G1=1
3193 G2=0
3195 GRG(X)=GG*G1+GR*G2+(1-G1-G2)*G0
3200 IF TT(X) <= TTR GOTO 3230
3210 CT=CT1*(TT(X)-TRT)/(CT2+TT(X)-TRT)
3215 Tag(X)=Tag0*10^(CT)
3220 GOTO 3250
3230 CT=-C3*(TT(X)-TRT)
3240 Tag(X)=Tag0*exp(CT)
3250 NAR(X)=GRG(X)*TAG(X)
3260 IF dT<-2.5*10^(-5) THEN 3275
3265 dT(X)=0
3270 dT=-2.5*10^(-5)
3272 goto 3290
3275 if dt>-170 then 3285
3278 dT(X)=dT
3280 dT=-170
3282 goto 3290
3285 DT(X)=DT
3290 TD=DT
3300 N(X)=0.8-0.0143*Log(-dT)
3350 TpS(X)=P(x,0)-S(X,0)
3370 Kg(X)=Kg0
3400 Kr(X)=Kr0
3410 Ka(X)=Ka0
3420 Ar(X)=Ar0

```

3430 Ag(X)=Ag0
3430 Aa(X)=Aa0
3500 TG(X)=TG0+ATG*(TpS(X)+abs(TpS(X)))/2
3510 if sw1=0 then 3590
3520 sw1=0
3530 return
3590 Vr(X)=VS0*(1-Kr(X)*(TpS(X)+abs(TpS(X)))/2)
3615 Vv(x)=Vr(x)*(1-ag(X)*(T0-TT(X)))
3625 TA(X)=1-U(0,X)/Vv(X)
3630 IF TA(X)>1*10^(-8) THEN 3650
3635 TA(X)=1*10^(-8)
3650 TAU(X)=TAU0*EXP(-BB*Ka0*(TpS(X)+abs(TpS(X)))/2)
3655 TAU(X)=TAU(X)*EXP(-Bb*(TA(X))^N(X))
3660 IF TT(X)>=TG(X) THEN 3685
3670 GF(X)=1
3675 FG(X)=1
3680 GOTO 3710
3685 FG(X)=0
3690 VG(X)=U(0,X)
3700 PG(X)=(TpS(X)+abs(TpS(X)))/2
3710 VE1=VR(X)*(1-AR(X)*(T0-TT(X)))
3720 VE2=VR(X)*(1-AR(X)*(T0-TG(X)))
3730 VE2=VE2*(1-AG(X)*(TG(X)-TT(X)))
3740 VE(X)=(1-FG(X))*VE1+FG(X)*VE2
3780 RETURN

```

3800 REM Subprogram for the constraint conditions

```

3810 if s > tc then 3825
3820 if s > tp then 3952
3822 REM during the packing step
3825 FOR G=TI TO L+1 STEP -1
3830 Q(CC,G)=Q(CC-1,G)
3835 D1W(G)=D1W(G)
3840 W(G)=W(G)
3845 NEXT G
3850 Q(CC,L)=Q(CC-1,L)+P
3855 D1W(L)=Q(CC,L)/ED
3860 W(L)=U(0,L)+Q(CC,L)
3865 FOR G=L-1 TO 1 STEP -1
3870 Q(CC,G)=Q(CC-1,G)
3875 D1W(G)=Q(CC,G)/ED

```

```

3880 W(G)=U(0,G)+Q(CC,G)
3885 NEXT G
3890 goto 4042
3950 REM during the cooling and post-ejection steps
3952 FOR G=TI TO L+1 STEP -1
3954 Q(CC,G)=Q(CC-1,G)
3956 D1W(G)=D1W(G)
3958 W(G)=W(G)
3960 NEXT G
3962 Q(CC,L)=Q(CC-1,L)+P
3964 D1W(L)=Q(CC,L)/ED
3966 W(L)=U(0,L)+Q(CC,L)
3968 FOR G=L-1 TO 1 STEP -1
3970 Q(CC,G)=Q(CC-1,G)-P/(L-1)
3972 D1W(G)=Q(CC,G)/ED
3974 W(G)=U(0,G)+Q(CC,G)
3976 NEXT G

4040 REM Subprogram for solving equations by the fourth-order
      Runge-Kutta method

4042 IF S > tc THEN 4050
4044 IF S < tp THEN 4050
4046 Lk=1
4048 goto 4055
4050 Lk=L
4055 FOR X=L TO Lk STEP -1
4060 FOR I=1 TO NF
4065 V(X,NF+I)=U(X,I)
4070 NEXT I
4075 GOSUB 5010
4080 FOR I=1 TO NF
4090 K(1,I)=F(X,I)
4100 NEXT I
4110 FOR Q=1 TO 3
4120 FOR I=1 TO NF
4130 V(X,I)=V(X,NF+I)+D1*K(Q,I)*INT(Q/3+1)
4140 NEXT I
4150 GOSUB 5010
4160 FOR I=1 TO NF
4170 K(Q+1,I)=F(X,I)
4180 NEXT I

```

```

4190 NEXT Q
4200 FOR I=1 TO NF
4210 V(X,I)=V(X,NF+I)+D1/3*(K(1,I)+K(4,I)+2*K(2,I)+2*K(3,I))
4220 NEXT I
4230 NEXT X
4233 for x=1 to Ti
4235 TpS(X)=P(x,0)-S(X,0)
4237 next x
4240 Tps=Tps(1)
4250 for x=2 to Ti
4260 if Tps(X) >= Tps then 4280
4270 Tps=Tps(x)
4280 next x
4310 Tps(0)=0
4320 for x=1 to Ti
4330 Tps(0)=Tps(0)+Tps(X)/(Ti )
4340 next x

4350 REM Subprogram for the force balance equations

4370 if s > tc then 4610
4390 if s<=tp then 4510
4410 SV=0
4420 FOR X=1 TO TI-1
4430 SV=SV+ABS(-V(X+1,1)+V(X,1)-V(X,2)+V(X+1,2))
4440 NEXT X
4450 FSV=ABS(SV)
4460 RETURN

4510 SV=0
4515 Pack=(46.6+2.5*s-1.77*s^2 +0.16145*s^3-0.0044*s^4)*10^6
4520 FOR X=1 TO TI
4530 SV=SV+ABS(V(X,1)-V(X,2)-Pack)
4540 NEXT X
4550 FSV=ABS(SV)
4560 RETURN

4610 SV=0
4720 if s > tc+.5 then 4728
4722 paging=(1-(s-tc)/.5)*7000000
4724 goto 4730
4728 Paging=0

```

```

4730 FOR X=1 TO TI
4732 SV=SV+ABS(V(X,1)-V(X,2)-Paging)
4736 next x
4750 fsv=(1+abs(sv))
4760 RETURN

```

```

5000 REM Coupling simulation equations

```

```

5010 F(X,1)=(VR(X)*Aa(X)*DT(X)-D1W(X)-(W(X)-
      VE(X))/TAU(X))/(VR(X)*Ka(X))
5550 F(X,2)=(4*GRG(X)/3+2*s(x,0))*D1W(X)/U(0,x)-s(x,0)/TAG(X)
5560 F(X,3)=(-2*GRG(X)/3)*D1W(X)/U(0,x)-T(x,6)/TAG(X)
5570 RETURN

```

```

6500 REM Data files

```

```

6510 PRINT #1,,k,,S,,P(1,0),P(2,0),P(3,0),P(4,0),P(5,0),
6515 PRINT #1,P(6,0),P(7,0),P(8,0),P(9,0),P(10,0)
6520 PRINT #2,,k,,S,,S(1,0),S(2,0),S(3,0),S(4,0),S(5,0),
6525 PRINT #2,S(6,0),S(7,0),S(8,0),S(9,0),S(10,0)
6530 PRINT #3,,k,,S,,T(1,4),T(2,4),T(3,4),T(4,4),T(5,4),
6535 PRINT #3,T(6,4),T(7,4),T(8,4),T(9,4),T(10,4)
6540 PRINT #4,,k,,S,,U(0,1),U(0,2),U(0,3),U(0,4),U(0,5),
6545 PRINT #4,U(0,6),U(0,7),U(0,8),U(0,9),U(0,10)
6550 PRINT #5,,k,,S,,T(1,1),T(2,1),T(3,1),T(4,1),T(5,1),
6555 PRINT #5,T(6,1),T(7,1),T(8,1),T(9,1),T(10,1)
6560 PRINT #6,,k,,S,,T(1,2),T(2,2),T(3,2),T(4,2),T(5,2),
6565 PRINT #6,T(6,2),T(7,2),T(8,2),T(9,2),T(10,2)
6570 PRINT #7,,k,,S,,T(1,3),T(2,3),T(3,3),T(4,3),T(5,3),
6575 PRINT #7,T(6,3),T(7,3),T(8,3),T(9,3),T(10,3)
6580 PRINT #8,,k,,S,,T(1,5),T(2,5),T(3,5),T(4,5),T(5,5),
6585 PRINT #8,T(6,5),T(7,5),T(8,5),T(9,5),T(10,5)
6590 PRINT #9,,k,,S,,T(1,6),T(2,6),T(3,6),T(4,6),T(5,6),
6595 PRINT #9,T(6,6),T(7,6),T(8,6),T(9,6),T(10,6)
6600 print #10,,k,,s,,1/u(0,1),1/u(0,2),1/u(0,3),1/u(0,4),1/u(0,5),
6605 print #10,1/u(0,6),1/u(0,7),1/u(0,8),1/u(0,9),1/u(0,10)
6607 print #11,k,s,T(10,4),tps(0),ad
6608 print #11,hx,hy,hz,tv,tm
6610 PRINT "S=";S,"CC=";CC,"k=";k,"u=";u
6612 PRINT "    TEMP(1)---TEMP(10)"
6614 PRINT T(1,5),T(2,5),T(3,5),T(4,5),T(5,5)

```

```

6616 PRINT T(6,5),T(7,5),T(8,5),T(9,5),T(10,5)
6620 PRINT "    TAU(1)---TAU(10)"
6622 PRINT T(1,1),T(2,1),T(3,1),T(4,1),T(5,1)
6625 PRINT T(6,1),T(7,1),T(8,1),T(9,1),T(10,1)
6630 PRINT "    P(1)---P(10)"
6640 PRINT P(1,0),P(2,0),P(3,0),P(4,0),P(5,0)
6645 PRINT P(6,0),P(7,0),P(8,0),P(9,0),P(10,0)
6650 PRINT "    Sy(1)---Sy(10)"
6660 PRINT S(1,0),S(2,0),S(3,0),S(4,0),S(5,0)
6665 PRINT S(6,0),S(7,0),S(8,0),S(9,0),S(10,0)
6670 PRINT "    ST(1)---ST(10)"
6680 PRINT T(1,4),T(2,4),T(3,4),T(4,4),T(5,4)
6685 PRINT T(6,4),T(7,4),T(8,4),T(9,4),T(10,4)
6690 PRINT "    D(1)---D(10)"
6700 PRINT 1/U(0,1),1/U(0,2),1/U(0,3),1/U(0,4),1/U(0,5)
6710 PRINT 1/U(0,6),1/U(0,7),1/U(0,8),1/U(0,9),1/U(0,10)
6720 PRINT "    Sx(1)---Sx(10)"
6760 PRINT T(1,6),T(2,6),T(3,6),T(4,6),T(5,6)
6765 PRINT T(6,6),T(7,6),T(8,6),T(9,6),T(10,6)
6770 PRINT "HX      HZ      TV      TM      AD"
6775 PRINT HX,HZ,TV,TM,AD
6790 PRINT
6800 RETURN

```

7000 REM Subprogram for giving initial values

```

7200 DY=H/TI
7210 FOR X=1 TO TI
7220 H(X)=(2*X-1)*H/2/TI
7222 P(X,0)=P0
7224 TpS(X)=P0
7226 S(X,0)=0
7230 sw1=1
7235 gosub 2220
7250 NEXT X
7255 sw1=1
7260 FOR X=1 TO TI
7264 V(X,1)=P0
7266 V(X,2)=0.0001
7270 V(X,3)=0.0001
7278 F(X,1)=-1000
7280 F(X,2)=10

```

```

7282 F(X,3)=10
7300 if TT(X)>Tg(X) then 7320
7305 Vr(X)=Vso*(1-ar(X)*(T0-Tg(X)))*(1-ag(X)*(Tg(x)-TT(X)))
7310 U(0,X)=Vr(X)*(1-Kg0*P0)
7313 Vv(X)=Vso*(1-ag(X)*(T0-TT(X)))*(1-Kg0*P0)
7316 GOTO 7324
7320 Vr(X)=Vso*(1-ar(X)*(T0-TT(X)))
7322 U(0,X)=Vr(X)*(1-Ka0*P0)
7323 Vv(X)=Vso*(1-ag(X)*(T0-TT(X)))*(1-Ka0*P0)
7324 TA(X)=1-U(0,X)/Vv(X)
7326 TA(X)=abs(TA(X))
7328 Vs(X)=U(0,X)
7330 GV(X)=U(0,X)
7331 D1U(0,X)=0
7332 FG(X)=0
7333 VG(X)=VS(X)
7334 U(X,0)=U(0,X)
7337 GF(X)=0
7360 IF TT(X)>=TG(X) THEN 7385
7370 GF(X)=1
7375 FG(X)=1
7380 GOTO 7410
7385 FG(X)=0
7390 VG(X)=U(0,X)
7400 PG(X)=TpS(X)
7410 VE1=VR(X)*(1-AR(X)*(T0-TT(X)))
7420 VE2=VR(X)*(1-AR(X)*(T0-TG(X)))
7430 VE2=VE2*(1-AG(X)*(TG(X)-TT(X)))
7440 VE(X)=(1-FG(X))*VE1+FG(X)*VE2
7445 TAU(X)=TAU0*EXP(-BB*Kr0*abs(TpS(X)))
7455 TAU(X)=TAU(X)*EXP(-Bb*(TA(X))^N(X))
7544 PF(X,0)=-1000
7546 S(X,0)=.0001
7548 VY(X)=0
7549 DVY(X)=0
7550 NEXT X

7555 FOR I=1 TO NF
7560 FOR Q=1 TO 4
7570 K(Q,I)=F(1,I)
7580 NEXT Q
7590 NEXT I

```

```

7600 FOR X=0 TO CN
7620 FOR Y=0 TO NL
7640 PF(X,Y)=0
7660 Q(X,Y)=0
7680 NEXT Y
7700 NEXT X
7710 for x=0 to Ti
7720 t(x,1)=tau(x)
7730 t(x,2)=Tag(x)
7740 t(x,3)=Nar(x)
7750 t(x,4)=P0
7760 t(x,5)=TT(X)
7770 t(x,6)=0.0001
7780 next x
7810 for x=1 to TI
7840 W(X)=U(0,x)
7860 U(x,0)=W(X)
7870 D1W(X)=0
7880 next x
7890 U(0,0)=W(1)
7900 Gosub 2000
7980 GOSUB 9710
7990 GOTO 580

```

8000 REM Subprogram for giving initial conditions and values

```

8010 H=.127
8020 T0=200
8025 TE=85
8040 OPT=.618
8050 IP=3.14159
8080 SV0=3.687
8085 Tv0=2*Sv0
8090 Vso=1.034
8095 Vs0=Vso
8100 V0=SV0/TI
8110 TTR=125
8120 TAU0=1.81*10(-8)
8130 TAG0=0.14676
8140 C3=.22
8150 Ag0=2.3*10(-4)
8160 Ar0=5.8*10(-4)

```

```
8170 Aa0=2.5*10^(-4)
8200 GG=1.5*10^9
8210 GR=2*10^5
8225 TG0=85
8250 S=1*10^(-9)
8255 sd=s
8260 DS=5*10^(-4)
8290 SV=0
8330 ATG=3.3*10^(-7)
8400 hy0=3.81
8410 hx0=7.62
8420 tv=2*sv0
8500 for x=1 to Ti
8510 TT(X)=T0
8520 next x
8600 CT1=-4.3
8610 CT2=80
8620 TRT=160
8888 GOTO 550
```

```
8910 FOR X=1 TO TI
8912 FOR Y=1 TO NF
8914 V(X,Y)=U(X,Y)
8916 NEXT Y
8918 NEXT X
8920 RETURN
```

```
9710 FOR X=1 TO TI
9720 FOR Y=1 TO NF
9730 U(X,Y)=V(X,Y)
9740 NEXT Y
9750 NEXT X
9760 RETURN
```

```
9900 REM End of the program
```

```
9910 CLOSE #1
9920 CLOSE #2
9930 CLOSE #3
9940 CLOSE #4
9950 CLOSE #5
9960 CLOSE #6
```

9970 CLOSE #7
9975 CLOSE #8
9980 CLOSE #9
9985 CLOSE #10
9990 CLOSE #11
9999 END

APPENDIX B

COMPUTER SIMULATION PROGRAM OF POST-FILLING STEPS FOR THE DELFT GROUP CASE

100 REM Computer Simulation Program of Post-Filling Steps for
 the Delft Group Case

122 OPEN "DGCP.dat" FOR OUTPUT AS #1
124 OPEN "DGCY.dat" FOR OUTPUT AS #2
126 OPEN "DGCS.dat" FOR OUTPUT AS #3
128 OPEN "DGCV.dat" FOR OUTPUT AS #4
130 OPEN "DGCO.dat" FOR OUTPUT AS #5
132 OPEN "DGCG.dat" FOR OUTPUT AS #6
134 OPEN "DGCR.dat" FOR OUTPUT AS #7
136 OPEN "DGCT.dat" FOR OUTPUT AS #8
138 OPEN "DGCX.dat" FOR OUTPUT AS #9
140 OPEN "DGCD.dat" FOR OUTPUT AS #10
142 OPEN "DGCB.dat" FOR OUTPUT AS #11

145 REM M0 is the terms of summation of heat transfer equation
 before mold opens

150 REM Ma is the terms of summation of heat transfer equation
 after mold opens

152 REM U0 is the control of time increment

154 REM TI is the number of layers of half thickness

156 REM Hk is for h_{tc}/k

158 REM NF is the number of simultaneous equations

160 REM AF is the thermal diffusivity

162 REM Ts is the starting temperature

164 REM Tw is the wall temperature

166 REM Tz is the initial temperature for post-ejection step

168 REM CN is the up limitation of iteration number

170 REM Kr0 is pressure compressibility coefficient of rubber state

172 REM Kg0 is pressure compressibility coefficient of glass state

174 REM Ka0 is the average pressure compressibility coefficient

176 REM P0 is the initial packing pressure

178 REM tp is the time point of the end of packing

180 REM tc is the time point of the end of cooling

182 REM NL is the limitation of data dimension

```

210 M0=60
215 Ma=26
225 U0=40
230 TI=10
235 Hk=4.762
240 Bb=-500
250 NF=3
270 AF=7*10^(-4)
275 Ts=200
280 Tw=50
285 Tz=70
300 CN=30
310 Kr0=9.3*10^(-10)
330 Ka0=7.3*10^(-10)
340 P0=4.2*10^7
350 Kg0=5.3*10^(-10)
360 tp=4
365 tc=15
370 NL=30
400 DIM N(TI),H(TI),TG(TI),FG(TI),GF(TI),iT(TI),Mv(TI)
410 DIM TT(TI),DT(TI),PP(NL),Q(CN,NL),PF(CN,NL)
420 DIM F(NL,NL),V(NL,NL),P(NL,NL),T(NL,NL),S(NL,NL)
430 DIM K(4,NL),FS(NL),DS(K0),TD(NL,K0),Tv(Ti),Tm(Ti)
440 DIM U(NL,Ti),W(NL),D1U(NL,NL),D1W(NL),EFA(NL),EFB(NL)
450 DIM Kr(NL),Kg(NL),Ar(NL),Ag(NL),TpS(NL),EFC(NL),EFD(NL)
460 DIM CC(K0,UK),NAR(NL),GRG(NL),DP(NL)
470 DIM PG(NL),GV(NL),VG(NL),DV(NL),Ka(NL)
480 DIM EV(NL),VE(NL),VR(NL),TA(NL),Aa(NL),Vv(NL)
490 DIM STR(NL),TAG(NL),TAU(NL),VY(NL),DVY(NL)

500 S0=10.65
510 S1=0.2
540 GOTO 8010
550 GOTO 7200
580 gosub 6500
620 FOR K=-5 TO 20 step 0.1
630 uu=int(U0/(abs(k)+2))
640 ED=(exp(k+0.1)-exp(k))/uu
645 D1=ED/2
650 U=1
652 FOR X=0 TO CN

```

```

653 FOR Y=0 TO NL
654 Q(X,Y)=0
655 PP(Y)=0
657 NEXT Y
658 NEXT X
663 S=s+ed
665 S1=S1+ed
667 S2=S2+ed
669 IF s>360 then 9910
670 FOR X=1 TO TI
680 GOSUB 2220
690 NEXT X
700 CC=0
710 cc=cc+1
715 if s > tc then 730
720 if S> tp then 750
730 Le=1
740 goto 760
750 Le=2
760 FOR L=TI TO Le STEP -1
770 GOSUB 1110
780 FOR Y1=1 TO TI
790 Q(CC-1,Y1)=Q(CC,Y1)
800 DV(Y1)=Q(CC,Y1)
810 NEXT Y1
815 NEXT L
816 IF s<tp then 820
817 IF ABS(F0)<1*100 THEN 824
818 goto 822
820 IF ABS(F0)<1*10^5 THEN 824
822 IF CC<CN THEN 710
824 GOSUB 9710
826 GOSUB 2010
830 if s > (tc+0.5) then 875
835 if s < (tc-0.5) then 875
840 gosub 6500
875 U=U+1
880 IF U<=Uu THEN 652
885 gosub 6500
890 NEXT K
900 GOTO 9910

```

```

1100 REM Subprogram of Optimization and Multimodal Searching
1110 P1=-0.03
1125 P2=0.03
1220 P=P1
1230 GOSUB 3810
1240 F1=FSV
1260 P=P2
1270 GOSUB 3810
1280 F2=FSV
1290 P3=P2-OPT*(P2-P1)
1300 P=P3
1310 GOSUB 3810
1320 F3=FSV
1330 P4=P1+OPT*(P2-P1)
1340 P=P4
1350 GOSUB 3810
1360 F4=FSV
1400 IF ABS(P2-P1)<5*10(-6) THEN 1600
1410 IF F3>=F4 THEN 1500
1420 P2=P4
1425 F2=F4
1430 P4=P3
1440 P3=P2-OPT*(P2-P1)
1450 F4=F3
1460 P=P3
1470 GOSUB 3810
1480 F3=FSV
1490 GOTO 1400
1500 P1=P3
1505 F1=F3
1510 P3=P4
1520 F3=F4
1530 GOTO 1330
1600 IF F3<=F4 THEN 1630
1610 PP(L)=P4
1615 F0=F4
1620 GOTO 1650
1630 PP(L)=P3
1640 F0=F3
1650 P=PP(L)
1655 GOSUB 3810
1660 RETURN

```

2000 REM Subprogram for storing iteration data

```
2010 FOR X=TI TO 1 STEP -1
2011 U(X,0)=U(0,X)
2012 U(0,X)=W(X)
2014 D1U(0,X)=D1W(X)
2030 P(X,0)=V(X,1)
2033 PF(X,0)=F(X,1)
2036 S(X,0)=V(X,2)
2064 T(X,1)=TAU(X)
2066 T(X,2)=TAG(X)
2068 T(X,3)=NAR(X)
2070 T(X,4)=P(X,0)-S(X,0)
2072 T(X,5)=TT(X)
2074 T(X,6)=V(X,3)
2076 NEXT X
2100 if s > tc then 2155
2105 REM for packing and cooling steps
2110 tm=0
2112 for x=1 to Ti
2114 tm(x)=V0/U(0,x)
2116 tm=tm+2*tm(X)
2118 next x
2120 hx=hx0
2124 hy=hy0
2128 hz=h*2
2130 ad=tm/sv0/2
2133 tv=2*sv0
2134 tm0=tm
2140 tv0=tv
2145 goto 2190
2150 REM for post-ejection step
2155 Tv=0
2157 for x=1 to Ti
2160 Tv(X)=tm(X)*U(0,x)
2165 tv=tv+2*tv(X)
2170 next x
2172 tm=tm0
2174 xyz=1+(tv-tv0)/3/tv0
2176 hx=hx*xyz
2178 hy=hy*xyz
```

```

2180 hz=hz*xyz
2182 ad=tm0/tv
2184 tv0=tv
2186 tm0=tm
2190 RETURN

```

2200 REM Subprogram for temperature

```

2220 if TT(X) > Tw then 2260
2230 TT(X)=Tw
2240 goto 3350
2260 if s > tc then 2440
2350 Ss=s1
2370 Tw=50
2390 S2=0
2400 goto 3010
2420 REM Temperature for the post-ejection step
2440 Ss=s2+S0
2470 Tw=-18
2540 T=0
2550 DT=0
2560 sm=1
2610 EFA(X)=0
2620 EFB(X)=0
2630 EFC(X)=0
2640 EFD(X)=0
2650 xa=(H-H(X))/(2*SQR(AF*Ss))
2660 xb=(H+H(X))/(2*SQR(AF*Ss))
2670 xc=hk*SQR(AF*Ss)+xa
2680 xd=hk*SQR(AF*Ss)+xb
2690 xe=hk*(H-H(X))+hk*hk*AF*Ss
2695 xf=hk*(H+H(X))+hk*hk*AF*Ss
2700 FOR m=0 TO Ma
2705 mm=1
2710 FOR mn=1 TO m
2720 mm=mm*mn
2730 NEXT mn
2740 EFA(X)=EFA(X)+(sm*(xa)^(2*m+1))/mm/(2*m+1)
2750 EFB(X)=EFB(X)+(sm*(xb)^(2*m+1))/mm/(2*m+1)
2760 EFC(X)=EFC(X)+(sm*(xc)^(2*m+1))/mm/(2*m+1)
2770 EFD(X)=EFD(X)+(sm*(xd)^(2*m+1))/mm/(2*m+1)
2780 sm=sm*(-1)

```

```

2790 NEXT m
2800 EFA(X)=1-2*EFA(X)/(SQR(IP))
2820 EFB(X)=1-2*EFB(X)/(SQR(IP))
2830 EFC(X)=1-2*EFC(X)/(SQR(IP))
2840 EFD(X)=1-2*EFD(X)/(SQR(IP))
2850 if TT(X)<=Tw then 2880
2860 Tm=1-EFA(X)-EFB(X)+EXP(xe)*EFC(X)+EXP(xf)*EFD(X)
2870 goto 2900
2880 Tm=0
2900 T=Tw+(Tz-Tw)*Tm
2940 IF T>Tz THEN 2980
2950 IF T>Tw THEN 2990
2960 T=Tw
2965 dt=0
2970 GOTO 2995
2980 T=Tz
2990 dT=(T-TT(X))/ed
2995 Goto 3135

3000 REM Temperature for the packing and cooling steps
3010 T=Tw
3020 DT=0
3030 SM=1
3040 FOR M=0 TO M0
3050 MPH=(M+.5)*IP/H
3060 Tm=2*(Ts-TW)*SM/MPH*COS(MPH*H(X))*EXP(-
    MPH*MPH*AF*Ss)/H
3070 T=T+TM
3080 DT=DT-MPH*MPH*AF*Tm
3090 Sm=Sm*(-1)
3100 NEXT M
3110 IF T>Ts THEN 3130
3115 IF T>Tw THEN 3135
3120 T=Tw
3125 GOTO 3135
3130 T=Ts
3135 TT(X)=T

```

```

3140 REM Subprogram for elastic modulus, parameters and
      constants

3143 IF TT(X)>120 THEN 3180
3146 IF TT(X)<80 THEN 3190
3150 G1=0
3155 G2=0
3160 IF Tt(X)>100 THEN 3170
3164 G0=-97959+3244.8*tt(X)-34.9*tt(X)*tt(X)+.123*tt(X)*tt(X)*tt(X)
3166 G0=G0*10^6
3168 GOTO 3195
3170 G0=10^(652-17*tt(X)+.149*tt(X)*tt(X)-.00044*tt(X)*tt(X)*tt(X))
3175 GOTO 3195
3180 G1=0
3183 G2=1
3186 GOTO 3195
3190 G1=1
3193 G2=0
3195 GRG(X)=GG*G1+GR*G2+(1-G1-G2)*G0
3200 IF TT(X) <= TTR GOTO 3230
3210 CT=CT1*(TT(X)-TRT)/(CT2+TT(X)-TRT)
3215 Tag(X)=Tag0*10^(CT)
3220 GOTO 3250
3230 CT=-C3*(TT(X)-TRT)
3240 Tag(X)=Tag0*exp(CT)
3250 NAR(X)=GRG(X)*TAG(X)
3260 IF dT<-2.5*10^(-5) THEN 3275
3265 dT(X)=0
3270 dT=-2.5*10^(-5)
3272 goto 3290
3275 if dt>-170 then 3285
3278 dT(X)=dT
3280 dT=-170
3282 goto 3290
3285 DT(X)=DT
3290 TD=DT
3300 N(X)=0.8-0.0143*Log(-dT)
3350 TpS(X)=P(x,0)-S(X,0)
3370 Kg(X)=Kg0
3400 Kr(X)=Kr0
3410 Ka(X)=Ka0
3420 Ar(X)=Ar0

```

```

3430 Ag(X)=Ag0
3430 Aa(X)=Aa0
3500 TG(X)=TG0+ATG*(TpS(X)+abs(TpS(X)))/2)
3510 if sw1=0 then 3590
3520 sw1=0
3530 return
3590 Vr(X)=VS0*(1-Kr(X)*(TpS(X)+abs(TpS(X)))/2)
3615 Vv(x)=Vr(x)*(1-ag(X)*(T0-TT(X)))
3625 TA(X)=1-U(0,X)/Vv(X)
3630 IF TA(X)>1*10^(-8) THEN 3650
3635 TA(X)=1*10^(-8)
3650 TAU(X)=TAU0*EXP(-BB*Ka0*(TpS(X)+abs(TpS(X)))/2)
3655 TAU(X)=TAU(X)*EXP(-Bb*(TA(X))^N(X))
3660 IF TT(X)>=TG(X) THEN 3685
3670 GF(X)=1
3675 FG(X)=1
3680 GOTO 3710
3685 FG(X)=0
3690 VG(X)=U(0,X)
3700 PG(X)=(TpS(X)+abs(TpS(X)))/2
3710 VE1=VR(X)*(1-AR(X)*(T0-TT(X)))
3720 VE2=VR(X)*(1-AR(X)*(T0-TG(X)))
3730 VE2=VE2*(1-AG(X)*(TG(X)-TT(X)))
3740 VE(X)=(1-FG(X))*VE1+FG(X)*VE2
3780 RETURN

```

3800 REM Subprogram for the constraint conditions

```

3810 if s > tc then 3825
3820 if s > tp then 3952
3822 REM during the packing step
3825 FOR G=TI TO L+1 STEP -1
3830 Q(CC,G)=Q(CC-1,G)
3835 D1W(G)=D1W(G)
3840 W(G)=W(G)
3845 NEXT G
3850 Q(CC,L)=Q(CC-1,L)+P
3855 D1W(L)=Q(CC,L)/ED
3860 W(L)=U(0,L)+Q(CC,L)
3865 FOR G=L-1 TO 1 STEP -1
3870 Q(CC,G)=Q(CC-1,G)
3875 D1W(G)=Q(CC,G)/ED

```

```

3880 W(G)=U(0,G)+Q(CC,G)
3885 NEXT G
3890 goto 4042
3950 REM during the cooling and post-ejection steps
3952 FOR G=TI TO L+1 STEP -1
3954 Q(CC,G)=Q(CC-1,G)
3956 D1W(G)=D1W(G)
3958 W(G)=W(G)
3960 NEXT G
3962 Q(CC,L)=Q(CC-1,L)+P
3964 D1W(L)=Q(CC,L)/ED
3966 W(L)=U(0,L)+Q(CC,L)
3968 FOR G=L-1 TO 1 STEP -1
3970 Q(CC,G)=Q(CC-1,G)-P/(L-1)
3972 D1W(G)=Q(CC,G)/ED
3974 W(G)=U(0,G)+Q(CC,G)
3976 NEXT G

4040 REM Subprogram for solving equations by the fourth-order
      Runge-Kutta method

4042 IF S > tc THEN 4050
4044 IF S < tp THEN 4050
4046 Lk=1
4048 goto 4055
4050 Lk=L
4055 FOR X=L TO Lk STEP -1
4060 FOR I=1 TO NF
4065 V(X,NF+I)=U(X,I)
4070 NEXT I
4075 GOSUB 5010
4080 FOR I=1 TO NF
4090 K(1,I)=F(X,I)
4100 NEXT I
4110 FOR Q=1 TO 3
4120 FOR I=1 TO NF
4130 V(X,I)=V(X,NF+I)+D1*K(Q,I)*INT(Q/3+1)
4140 NEXT I
4150 GOSUB 5010
4160 FOR I=1 TO NF
4170 K(Q+1,I)=F(X,I)
4180 NEXT I

```

```

4190 NEXT Q
4200 FOR I=1 TO NF
4210 V(X,I)=V(X,NF+I)+D1/3*(K(1,I)+K(4,I)+2*K(2,I)+2*K(3,I))
4220 NEXT I
4230 NEXT X
4233 for x=1 to Ti
4235 TpS(X)=P(x,0)-S(X,0)
4237 next x
4240 Tps=Tps(1)
4250 for x=2 to Ti
4260 if Tps(X) >= Tps then 4280
4270 Tps=Tps(x)
4280 next x
4310 Tps(0)=0
4320 for x=1 to Ti
4330 Tps(0)=Tps(0)+Tps(X)/(Ti )
4340 next x

4350 REM Subprogram for the force balance equations

4370 if s > tc then 4610
4390 if s<=tp then 4510
4410 SV=0
4420 FOR X=1 TO TI-1
4430 SV=SV+ABS(-V(X+1,1)+V(X,1)-V(X,2)+V(X+1,2))
4440 NEXT X
4450 FSV=ABS(SV)
4460 RETURN

4510 SV=0
4515 Pack=(42+2.5*s-1.773*s^2 +0.16145*s^3-0.0044*s^4)*10^6
4520 FOR X=1 TO TI
4530 SV=SV+ABS(V(X,1)-V(X,2)-Pack)
4540 NEXT X
4550 FSV=ABS(SV)
4560 RETURN

4610 SV=0
4720 if s > tc+.5 then 4728
4722 paging=(1-(s-tc)/.5)*6000000
4724 goto 4730
4728 Paging=0

```

```

4730 FOR X=1 TO TI
4732 SV=SV+ABS(V(X,1)-V(X,2)-Paging)
4736 next x
4750 fsv=(1+abs(sv))
4760 RETURN

5000 REM Coupling simulation equations

5010 F(X,1)=(VR(X)*Aa(X)*DT(X)-D1W(X)-(W(X)-
      VE(X))/TAU(X))/(VR(X)*Ka(X))
5550 F(X,2)=(4*GRG(X)/3+2*s(x,0))*D1W(X)/U(0,x)-s(x,0)/TAG(X)
5560 F(X,3)=(-2*GRG(X)/3)*D1W(X)/U(0,x)-T(x,6)/TAG(X)
5570 RETURN

6500 REM Data files

6510 PRINT #1,,k,,S,,P(1,0),P(2,0),P(3,0),P(4,0),P(5,0),
6515 PRINT #1,P(6,0),P(7,0),P(8,0),P(9,0),P(10,0)
6520 PRINT #2,,k,,S,,S(1,0),S(2,0),S(3,0),S(4,0),S(5,0),
6525 PRINT #2,S(6,0),S(7,0),S(8,0),S(9,0),S(10,0)
6530 PRINT #3,,k,,S,,T(1,4),T(2,4),T(3,4),T(4,4),T(5,4),
6535 PRINT #3,T(6,4),T(7,4),T(8,4),T(9,4),T(10,4)
6540 PRINT #4,,k,,S,,U(0,1),U(0,2),U(0,3),U(0,4),U(0,5),
6545 PRINT #4,U(0,6),U(0,7),U(0,8),U(0,9),U(0,10)
6550 PRINT #5,,k,,S,,T(1,1),T(2,1),T(3,1),T(4,1),T(5,1),
6555 PRINT #5,T(6,1),T(7,1),T(8,1),T(9,1),T(10,1)
6560 PRINT #6,,k,,S,,T(1,2),T(2,2),T(3,2),T(4,2),T(5,2),
6565 PRINT #6,T(6,2),T(7,2),T(8,2),T(9,2),T(10,2)
6570 PRINT #7,,k,,S,,T(1,3),T(2,3),T(3,3),T(4,3),T(5,3),
6575 PRINT #7,T(6,3),T(7,3),T(8,3),T(9,3),T(10,3)
6580 PRINT #8,,k,,S,,T(1,5),T(2,5),T(3,5),T(4,5),T(5,5),
6585 PRINT #8,T(6,5),T(7,5),T(8,5),T(9,5),T(10,5)
6590 PRINT #9,,k,,S,,T(1,6),T(2,6),T(3,6),T(4,6),T(5,6),
6595 PRINT #9,T(6,6),T(7,6),T(8,6),T(9,6),T(10,6)
6600 print #10,,k,,s,,1/u(0,1),1/u(0,2),1/u(0,3),1/u(0,4),1/u(0,5),
6605 print #10,1/u(0,6),1/u(0,7),1/u(0,8),1/u(0,9),1/u(0,10)
6607 print #11,k,s,T(10,4),tps(0),ad
6608 print #11,hx,hy,hz,tv,tm
6610 PRINT "S=";S,"CC=";CC,"k=";k,"u=";u
6612 PRINT " TEMP(1)---TEMP(10)"
6614 PRINT T(1,5),T(2,5),T(3,5),T(4,5),T(5,5)

```

```

6616 PRINT T(6,5),T(7,5),T(8,5),T(9,5),T(10,5)
6620 PRINT "    TAU(1)---TAU(10)"
6622 PRINT T(1,1),T(2,1),T(3,1),T(4,1),T(5,1)
6625 PRINT T(6,1),T(7,1),T(8,1),T(9,1),T(10,1)
6630 PRINT "    P(1)---P(10)"
6640 PRINT P(1,0),P(2,0),P(3,0),P(4,0),P(5,0)
6645 PRINT P(6,0),P(7,0),P(8,0),P(9,0),P(10,0)
6650 PRINT "    Sy(1)---Sy(10)"
6660 PRINT S(1,0),S(2,0),S(3,0),S(4,0),S(5,0)
6665 PRINT S(6,0),S(7,0),S(8,0),S(9,0),S(10,0)
6670 PRINT "    ST(1)---ST(10)"
6680 PRINT T(1,4),T(2,4),T(3,4),T(4,4),T(5,4)
6685 PRINT T(6,4),T(7,4),T(8,4),T(9,4),T(10,4)
6690 PRINT "    D(1)---D(10)"
6700 PRINT 1/U(0,1),1/U(0,2),1/U(0,3),1/U(0,4),1/U(0,5)
6710 PRINT 1/U(0,6),1/U(0,7),1/U(0,8),1/U(0,9),1/U(0,10)
6720 PRINT "    Sx(1)---Sx(10)"
6760 PRINT T(1,6),T(2,6),T(3,6),T(4,6),T(5,6)
6765 PRINT T(6,6),T(7,6),T(8,6),T(9,6),T(10,6)
6770 PRINT "HX      HZ      TV      TM      AD"
6775 PRINT HX,HZ,TV,TM,AD
6790 PRINT
6800 RETURN

```

7000 REM Subprogram for giving initial values

```

7200 DY=H/TI
7210 FOR X=1 TO TI
7220 H(X)=(2*X-1)*H/2/TI
7222 P(X,0)=P0
7224 TpS(X)=P0
7226 S(X,0)=0
7230 sw1=1
7235 gosub 2220
7250 NEXT X
7255 sw1=1
7260 FOR X=1 TO TI
7264 V(X,1)=P0
7266 V(X,2)=0.0001
7270 V(X,3)=0.0001
7278 F(X,1)=-1000
7280 F(X,2)=10

```

```

7282 F(X,3)=10
7300 if TT(X)>Tg(X) then 7320
7305 Vr(X)=Vso*(1-ar(X)*(T0-Tg(X)))*(1-ag(X)*(Tg(x)-TT(X)))
7310 U(0,X)=Vr(X)*(1-Kg0*P0)
7313 Vv(X)=Vso*(1-ag(X)*(T0-TT(X)))*(1-Kg0*P0)
7316 GOTO 7324
7320 Vr(X)=Vso*(1-ar(X)*(T0-TT(X)))
7322 U(0,X)=Vr(X)*(1-Ka0*P0)
7323 Vv(X)=Vso*(1-ag(X)*(T0-TT(X)))*(1-Ka0*P0)
7324 TA(X)=1-U(0,X)/Vv(X)
7326 TA(X)=abs(TA(X))
7328 Vs(X)=U(0,X)
7330 GV(X)=U(0,X)
7331 D1U(0,X)=0
7332 FG(X)=0
7333 VG(X)=VS(X)
7334 U(X,0)=U(0,X)
7337 GF(X)=0
7360 IF TT(X)>=TG(X) THEN 7385
7370 GF(X)=1
7375 FG(X)=1
7380 GOTO 7410
7385 FG(X)=0
7390 VG(X)=U(0,X)
7400 PG(X)=TpS(X)
7410 VE1=VR(X)*(1-AR(X)*(T0-TT(X)))
7420 VE2=VR(X)*(1-AR(X)*(T0-TG(X)))
7430 VE2=VE2*(1-AG(X)*(TG(X)-TT(X)))
7440 VE(X)=(1-FG(X))*VE1+FG(X)*VE2
7445 TAU(X)=TAU0*EXP(-BB*Kr0*abs(TpS(X)))
7455 TAU(X)=TAU(X)*EXP(-BF*(TA(X))^N(X))
7544 PF(X,0)=-1000
7546 S(X,0)=.0001
7548 VY(X)=0
7549 DVY(X)=0
7550 NEXT X

7555 FOR I=1 TO NF
7560 FOR Q=1 TO 4
7570 K(Q,I)=F(1,I)
7580 NEXT Q
7590 NEXT I

```

```

7600 FOR X=0 TO CN
7620 FOR Y=0 TO NL
7640 PF(X,Y)=0
7660 Q(X,Y)=0
7680 NEXT Y
7700 NEXT X
7710 for x=0 to Ti
7720 t(x,1)=tau(x)
7730 t(x,2)=Tag(x)
7740 t(x,3)=Nar(x)
7750 t(x,4)=P0
7760 t(x,5)=TT(X)
7770 t(x,6)=0.0001
7780 next x
7810 for x=1 to TI
7840 W(X)=U(0,x)
7860 U(x,0)=W(X)
7870 D1W(X)=0
7880 next x
7890 U(0,0)=W(1)
7900 Gosub 2000
7980 GOSUB 9710
7990 GOTO 580

```

```

8000 REM Subprogram for giving initial conditions and values

```

```

8010 H=.1
8020 T0=200
8025 TE=85
8040 OPT=.618
8050 IP=3.14159
8080 SV0=2.8
8085 Tv0=2*Sv0
8090 Vso=1.034
8095 Vs0=Vso
8100 V0=SV0/TI
8110 TTR=125
8120 TAU0=1.81*10(-8)
8130 TAG0=0.14676
8140 C3=.22
8150 Ag0=2.3*10(-4)
8160 Ar0=5.8*10(-4)

```

```

8170 Aa0=2.5*10^(-4)
8200 GG=1.5*10^9
8210 GR=2*10^5
8225 TG0=85
8250 S=1*10^(-9)
8255 sd=s
8260 DS=5*10^(-4)
8290 SV=0
8330 ATG=3.3*10^(-7)
8400 hy0=3.5
8410 hx0=8
8420 tv=2*sv0
8500 for x=1 to Ti
8510 TT(X)=T0
8520 next x
8600 CT1=-4.3
8610 CT2=80
8620 TRT=160
8888 GOTO 550

```

```

8910 FOR X=1 TO TI
8912 FOR Y=1 TO NF
8914 V(X,Y)=U(X,Y)
8916 NEXT Y
8918 NEXT X
8920 RETURN

```

```

9710 FOR X=1 TO TI
9720 FOR Y=1 TO NF
9730 U(X,Y)=V(X,Y)
9740 NEXT Y
9750 NEXT X
9760 RETURN

```

```

9900 REM End of the program

```

```

9910 CLOSE #1
9920 CLOSE #2
9930 CLOSE #3
9940 CLOSE #4
9950 CLOSE #5
9960 CLOSE #6

```

9970 CLOSE #7
9975 CLOSE #8
9980 CLOSE #9
9985 CLOSE #10
9990 CLOSE #11
9999 END

APPENDIX C

COMPUTER SIMULATION PROGRAM OF POST-FILLING STEPS FOR THE EINDHOVEN GROUP CASE

```
100 REM      Computer Simulation Program of Post-Filling Steps for
              the Eindhoven Group Case

122 OPEN "EGCP.dat" FOR OUTPUT AS #1
124 OPEN "EGCY.dat" FOR OUTPUT AS #2
126 OPEN "EGCS.dat" FOR OUTPUT AS #3
128 OPEN "EGCV.dat" FOR OUTPUT AS #4
130 OPEN "EGCO.dat" FOR OUTPUT AS #5
132 OPEN "EGCG.dat" FOR OUTPUT AS #6
134 OPEN "EGCR.dat" FOR OUTPUT AS #7
136 OPEN "EGCT.dat" FOR OUTPUT AS #8
138 OPEN "EGCX.dat" FOR OUTPUT AS #9
140 OPEN "EGCD.dat" FOR OUTPUT AS #10
142 OPEN "EGCb.dat" FOR OUTPUT AS #11

145 REM M0 is the terms of summation of heat transfer equation
      before mold opens
150 REM Ma is the terms of summation of heat transfer equation
      after mold opens
152 REM U0 is the control of time increment
154 REM TI is the number of layers of half thickness
156 REM Hk is for  $h_{tc}/k$ 
158 REM NF is the number of simultaneous equations
160 REM AF is the thermal diffusivity
162 REM Ts is the starting temperature
164 REM Tw is the wall temperature
166 REM Tz is the initial temperature for post-ejection step
168 REM CN is the up limitation of iteration number
170 REM Kr0 is pressure compressibility coefficient of rubber state
172 REM Kg0 is pressure compressibility coefficient of glass state
174 REM Ka0 is the average pressure compressibility coefficient
176 REM P0 is the initial packing pressure
178 REM tp is the time point of the end of packing
180 REM tc is the time point of the end of cooling
182 REM NL is the limitation of data dimension
```

```

210 M0=60
215 Ma=26
225 U0=40
230 TI=10
235 Hk=4.762
240 Bb=-500
250 NF=3
270 AF=7*10^(-4)
275 Ts=200
280 Tw=50
285 Tz=70
300 CN=30
310 Kr0=9.3*10^(-10)
330 Ka0=7.3*10^(-10)
340 P0=7.8*10^7
350 Kg0=5.3*10^(-10)
360 tp=2
365 tc=19
370 NL=30
400 DIM N(TI),H(TI),TG(TI),FG(TI),GF(TI),iT(TI),Mv(TI)
410 DIM TT(TI),DT(TI),PP(NL),Q(CN,NL),PF(CN,NL)
420 DIM F(NL,NL),V(NL,NL),P(NL,NL),T(NL,NL),S(NL,NL)
430 DIM K(4,NL),FS(NL),DS(K0),TD(NL,K0),Tv(Ti),Tm(Ti)
440 DIM U(NL,Ti),W(NL),D1U(NL,NL),D1W(NL),EFA(NL),EFB(NL)
450 DIM Kr(NL),Kg(NL),Ar(NL),Ag(NL),TpS(NL),EFC(NL),EFD(NL)
460 DIM CC(K0,UK),NAR(NL),GRG(NL),DP(NL)
470 DIM PG(NL),GV(NL),VG(NL),DV(NL),Ka(NL)
480 DIM EV(NL),VE(NL),VR(NL),TA(NL),Aa(NL),Vv(NL)
490 DIM STR(NL),TAG(NL),TAU(NL),VY(NL),DVY(NL)

500 S0=14.28
510 S1=0.2
540 GOTO 8010
550 GOTO 7200
580 gosub 6500
620 FOR K=-5 TO 20 step 0.1
630 uu=int(U0/(abs(k)+2))
640 ED=(exp(k+0.1)-exp(k))/uu
645 D1=ED/2
650 U=1
652 FOR X=0 TO CN

```

```

653 FOR Y=0 TO NL
654 Q(X,Y)=0
655 PP(Y)=0
657 NEXT Y
658 NEXT X
663 S=s+ed
665 S1=S1+ed
667 S2=S2+ed
669 IF s>360 then 9910
670 FOR X=1 TO TI
680 GOSUB 2220
690 NEXT X
700 CC=0
710 cc=cc+1
715 if s > tc then 730
720 if S> tp then 750
730 Le=1
740 goto 760
750 Le=2
760 FOR L=TI TO Le STEP -1
770 GOSUB 1110
780 FOR Y1=1 TO TI
790 Q(CC-1,Y1)=Q(CC,Y1)
800 DV(Y1)=Q(CC,Y1)
810 NEXT Y1
815 NEXT L
816 IF s<=tc then 820
817 IF ABS(F0)<1*100 THEN 824
818 goto 822
820 IF ABS(F0)<1*10^5 THEN 824
822 IF CC<CN THEN 710
824 GOSUB 9710
826 GOSUB 2010
830 if s > (tc+0.5) then 875
835 if s < (tc-0.5) then 875
840 gosub 6500
875 U=U+1
880 IF U<=Uu THEN 652
885 gosub 6500
890 NEXT K
900 GOTO 9910

```

```

1100 REM  Subprogram of Optimization and Multimodal Searching
1110 P1=-0.03
1125 P2=0.03
1220 P=P1
1230 GOSUB 3810
1240 F1=FSV
1260 P=P2
1270 GOSUB 3810
1280 F2=FSV
1290 P3=P2-OPT*(P2-P1)
1300 P=P3
1310 GOSUB 3810
1320 F3=FSV
1330 P4=P1+OPT*(P2-P1)
1340 P=P4
1350 GOSUB 3810
1360 F4=FSV
1400 IF ABS(P2-P1)<5*10(-6) THEN 1600
1410 IF F3>=F4 THEN 1500
1420 P2=P4
1425 F2=F4
1430 P4=P3
1440 P3=P2-OPT*(P2-P1)
1450 F4=F3
1460 P=P3
1470 GOSUB 3810
1480 F3=FSV
1490 GOTO 1400
1500 P1=P3
1505 F1=F3
1510 P3=P4
1520 F3=F4
1530 GOTO 1330
1600 IF F3<=F4 THEN 1630
1610 PP(L)=P4
1615 F0=F4
1620 GOTO 1650
1630 PP(L)=P3
1640 F0=F3
1650 P=PP(L)
1655 GOSUB 3810
1660 RETURN

```

2000 REM Subprogram for storing iteration data

```
2010 FOR X=TI TO 1 STEP -1
2011 U(X,0)=U(0,X)
2012 U(0,X)=W(X)
2014 D1U(0,X)=D1W(X)
2030 P(X,0)=V(X,1)
2033 PF(X,0)=F(X,1)
2036 S(X,0)=V(X,2)
2064 T(X,1)=TAU(X)
2066 T(X,2)=TAG(X)
2068 T(X,3)=NAR(X)
2070 T(X,4)=P(X,0)-S(X,0)
2072 T(X,5)=TT(X)
2074 T(X,6)=V(X,3)
2076 NEXT X
2100 if s > tc then 2155
2105 REM for packing and cooling steps
2110 tm=0
2112 for x=1 to Ti
2114 tm(x)=V0/U(0,x)
2116 tm=tm+2*tm(X)
2118 next x
2120 hx=hx0
2124 hy=hy0
2128 hz=h*2
2130 ad=tm/sv0/2
2133 tv=2*sv0
2134 tm0=tm
2140 tv0=tv
2145 goto 2190
2150 REM for post-ejection step
2155 Tv=0
2157 for x=1 to Ti
2160 Tv(X)=tm(X)*U(0,x)
2165 tv=tv+2*tv(X)
2170 next x
2172 tm=tm0
2174 xyz=1+(tv-tv0)/3/tv0
2176 hx=hx*xyz
2178 hy=hy*xyz
```

```

2180 hz=hz*xyz
2182 ad=tm0/tv
2184 tv0=tv
2186 tm0=tm
2190 RETURN

```

```

2200 REM Subprogram for temperature

```

```

2220 if TT(X) > Tw then 2260
2230 TT(X)=Tw
2240 goto 3350
2260 if s > tc then 2440
2350 Ss=s1
2370 Tw=50
2390 S2=0
2400 goto 3010
2420 REM Temperature for the post-ejection step
2440 Ss=s2+S0
2470 Tw=23
2540 T=0
2550 DT=0
2560 sm=1
2610 EFA(X)=0
2620 EFB(X)=0
2630 EFC(X)=0
2640 EFD(X)=0
2650 xa=(H-H(X))/(2*SQR(AF*Ss))
2660 xb=(H+H(X))/(2*SQR(AF*Ss))
2670 xc=hk*SQR(AF*Ss)+xa
2680 xd=hk*SQR(AF*Ss)+xb
2690 xe=hk*(H-H(X))+hk*hk*AF*Ss
2695 xf=hk*(H+H(X))+hk*hk*AF*Ss
2700 FOR m=0 TO Ma
2705 mm=1
2710 FOR mn=1 TO m
2720 mm=mm*mn
2730 NEXT mn
2740 EFA(X)=EFA(X)+(sm*(xa)^(2*m+1))/mm/(2*m+1)
2750 EFB(X)=EFB(X)+(sm*(xb)^(2*m+1))/mm/(2*m+1)
2760 EFC(X)=EFC(X)+(sm*(xc)^(2*m+1))/mm/(2*m+1)
2770 EFD(X)=EFD(X)+(sm*(xd)^(2*m+1))/mm/(2*m+1)
2780 sm=sm*(-1)

```

```

2790 NEXT m
2800 EFA(X)=1-2*EFA(X)/(SQR(IP))
2820 EFB(X)=1-2*EFB(X)/(SQR(IP))
2830 EFC(X)=1-2*EFC(X)/(SQR(IP))
2840 EFD(X)=1-2*EFD(X)/(SQR(IP))
2850 if TT(X)<=Tw then 2880
2860 Tm=1-EFA(X)-EFB(X)+EXP(xe)*EFC(X)+EXP(xf)*EFD(X)
2870 goto 2900
2880 Tm=0
2900 T=Tw+(Tz-Tw)*Tm
2940 IF T>Tz THEN 2980
2950 IF T>Tw THEN 2990
2960 T=Tw
2965 dt=0
2970 GOTO 2995
2980 T=Tz
2990 dT=(T-TT(X))/ed
2995 Goto 3135

3000 REM Temperature for the packing and cooling steps
3010 T=Tw
3020 DT=0
3030 SM=1
3040 FOR M=0 TO M0
3050 MPH=(M+.5)*IP/H
3060 Tm=2*(Ts-TW)*SM/MPH*COS(MPH*H(X))*EXP(-
      MPH*MPH*AF*Ss)/H
3070 T=T+TM
3080 DT=DT-MPH*MPH*AF*Tm
3090 Sm=Sm*(-1)
3100 NEXT M
3110 IF T>Ts THEN 3130
3115 IF T>Tw THEN 3135
3120 T=Tw
3125 GOTO 3135
3130 T=Ts
3135 TT(X)=T

```

```

3140 REM Subprogram for elastic modulus, parameters and
      constants

3143 IF TT(X)>120 THEN 3180
3146 IF TT(X)<80 THEN 3190
3150 G1=0
3155 G2=0
3160 IF Tt(X)>100 THEN 3170
3164 G0=-97959+3244.8*tt(X)-34.9*tt(X)*tt(X)+.123*tt(X)*tt(X)*tt(X)
3166 G0=G0*10^6
3168 GOTO 3195
3170 G0=10^(652-17*tt(X)+.149*tt(X)*tt(X)-.00044*tt(X)*tt(X)*tt(X))
3175 GOTO 3195
3180 G1=0
3183 G2=1
3186 GOTO 3195
3190 G1=1
3193 G2=0
3195 GRG(X)=GG*G1+GR*G2+(1-G1-G2)*G0
3200 IF TT(X) <= TTR GOTO 3230
3210 CT=CT1*(TT(X)-TRT)/(CT2+TT(X)-TRT)
3215 Tag(X)=Tag0*10^(CT)
3220 GOTO 3250
3230 CT=-C3*(TT(X)-TRT)
3240 Tag(X)=Tag0*exp(CT)
3250 NAR(X)=GRG(X)*TAG(X)
3260 IF dT<-2.5*10^(-5) THEN 3275
3265 dT(X)=0
3270 dT=-2.5*10^(-5)
3272 goto 3290
3275 if dt>-170 then 3285
3278 dT(X)=dT
3280 dT=-170
3282 goto 3290
3285 DT(X)=DT
3290 TD=DT
3300 N(X)=0.8-0.0143*Log(-dT)
3350 TpS(X)=P(x,0)-S(X,0)
3370 Kg(X)=Kg0
3400 Kr(X)=Kr0
3410 Ka(X)=Ka0
3420 Ar(X)=Ar0

```

```

3430 Ag(X)=Ag0
3430 Aa(X)=Aa0
3500 TG(X)=TG0+ATG*(TpS(X)+abs(TpS(X)))/2)
3510 if sw1=0 then 3590
3520 sw1=0
3530 return
3590 Vr(X)=VS0*(1-Kr(X)*(TpS(X)+abs(TpS(X)))/2)
3615 Vv(x)=Vr(x)*(1-ag(X)*(T0-TT(X)))
3625 TA(X)=1-U(0,X)/Vv(X)
3630 IF TA(X)>1*10^(-8) THEN 3650
3635 TA(X)=1*10^(-8)
3650 TAU(X)=TAU0*EXP(-BB*Ka0*(TpS(X)+abs(TpS(X)))/2)
3655 TAU(X)=TAU(X)*EXP(-Bb*(TA(X))^N(X))
3660 IF TT(X)>=TG(X) THEN 3685
3670 GF(X)=1
3675 FG(X)=1
3680 GOTO 3710
3685 FG(X)=0
3690 VG(X)=U(0,X)
3700 PG(X)=(TpS(X)+abs(TpS(X)))/2
3710 VE1=VR(X)*(1-AR(X)*(T0-TT(X)))
3720 VE2=VR(X)*(1-AR(X)*(T0-TG(X)))
3730 VE2=VE2*(1-AG(X)*(TG(X)-TT(X)))
3740 VE(X)=(1-FG(X))*VE1+FG(X)*VE2
3780 RETURN

```

3800 REM Subprogram for the constraint conditions

```

3810 if s > tc then 3825
3820 if s > tp then 3952
3822 REM during the packing step
3825 FOR G=TI TO L+1 STEP -1
3830 Q(CC,G)=Q(CC-1,G)
3835 D1W(G)=D1W(G)
3840 W(G)=W(G)
3845 NEXT G
3850 Q(CC,L)=Q(CC-1,L)+P
3855 D1W(L)=Q(CC,L)/ED
3860 W(L)=U(0,L)+Q(CC,L)
3865 FOR G=L-1 TO 1 STEP -1
3870 Q(CC,G)=Q(CC-1,G)
3875 D1W(G)=Q(CC,G)/ED

```

```

3880 W(G)=U(0,G)+Q(CC,G)
3885 NEXT G
3890 goto 4042
3950 REM during the cooling and post-ejection steps
3952 FOR G=TI TO L+1 STEP -1
3954 Q(CC,G)=Q(CC-1,G)
3956 D1W(G)=D1W(G)
3958 W(G)=W(G)
3960 NEXT G
3962 Q(CC,L)=Q(CC-1,L)+P
3964 D1W(L)=Q(CC,L)/ED
3966 W(L)=U(0,L)+Q(CC,L)
3968 FOR G=L-1 TO 1 STEP -1
3970 Q(CC,G)=Q(CC-1,G)-P/(L-1)
3972 D1W(G)=Q(CC,G)/ED
3974 W(G)=U(0,G)+Q(CC,G)
3976 NEXT G

```

```

4040 REM Subprogram for solving equations by the fourth-order
      Runge-Kutta method

```

```

4042 IF S > tc THEN 4050
4044 IF S < tp THEN 4050
4046 Lk=1
4048 goto 4055
4050 Lk=L
4055 FOR X=L TO Lk STEP -1
4060 FOR I=1 TO NF
4065 V(X,NF+I)=U(X,I)
4070 NEXT I
4075 GOSUB 5010
4080 FOR I=1 TO NF
4090 K(1,I)=F(X,I)
4100 NEXT I
4110 FOR Q=1 TO 3
4120 FOR I=1 TO NF
4130 V(X,I)=V(X,NF+I)+D1*K(Q,I)*INT(Q/3+1)
4140 NEXT I
4150 GOSUB 5010
4160 FOR I=1 TO NF
4170 K(Q+1,I)=F(X,I)
4180 NEXT I

```

```

4190 NEXT Q
4200 FOR I=1 TO NF
4210 V(X,I)=V(X,NF+I)+D1/3*(K(1,I)+K(4,I)+2*K(2,I)+2*K(3,I))
4220 NEXT I
4230 NEXT X
4233 for x=1 to Ti
4235 TpS(X)=P(x,0)-S(X,0)
4237 next x
4240 Tps=Tps(1)
4250 for x=2 to Ti
4260 if Tps(X) >= Tps then 4280
4270 Tps=Tps(x)
4280 next x
4310 Tps(0)=0
4320 for x=1 to Ti
4330 Tps(0)=Tps(0)+Tps(X)/(Ti )
4340 next x

4350 REM Subprogram for the force balance equations

4370 if s > tc then 4610
4390 if s<=tp then 4510
4410 SV=0
4420 FOR X=1 TO TI-1
4430 SV=SV+ABS(-V(X+1,1)+V(X,1)-V(X,2)+V(X+1,2))
4440 NEXT X
4450 FSV=ABS(SV)
4460 RETURN

4510 SV=0
4515 Pack=(77.13+4.77*s-3.865*s^2 +0.578*s^3-0.00283*s^4)*10^6
4520 FOR X=1 TO TI
4530 SV=SV+ABS(V(X,1)-V(X,2)-Pack)
4540 NEXT X
4550 FSV=ABS(SV)
4560 RETURN

4610 SV=0
4720 if s > tc+.5 then 4728
4722 paging=(1-(s-tc)/.5)*6000000
4724 goto 4730
4728 Paging=0

```

```

4730 FOR X=1 TO TI
4732 SV=SV+ABS(V(X,1)-V(X,2)-Paging)
4736 next x
4750 fsv=(1+abs(sv))
4760 RETURN

5000 REM Coupling simulation equations

5010 F(X,1)=(VR(X)*Aa(X)*DT(X)-D1W(X)-(W(X)-
      VE(X))/TAU(X))/(VR(X)*Ka(X))
5550 F(X,2)=(4*GRG(X)/3+2*s(x,0))*D1W(X)/U(0,x)-s(x,0)/TAG(X)
5560 F(X,3)=(-2*GRG(X)/3)*D1W(X)/U(0,x)-T(x,6)/TAG(X)
5570 RETURN

6500 REM Data files

6510 PRINT #1,,k,,S,,P(1,0),P(2,0),P(3,0),P(4,0),P(5,0),
6515 PRINT #1,P(6,0),P(7,0),P(8,0),P(9,0),P(10,0)
6520 PRINT #2,,k,,S,,S(1,0),S(2,0),S(3,0),S(4,0),S(5,0),
6525 PRINT #2,S(6,0),S(7,0),S(8,0),S(9,0),S(10,0)
6530 PRINT #3,,k,,S,,T(1,4),T(2,4),T(3,4),T(4,4),T(5,4),
6535 PRINT #3,T(6,4),T(7,4),T(8,4),T(9,4),T(10,4)
6540 PRINT #4,,k,,S,,U(0,1),U(0,2),U(0,3),U(0,4),U(0,5),
6545 PRINT #4,U(0,6),U(0,7),U(0,8),U(0,9),U(0,10)
6550 PRINT #5,,k,,S,,T(1,1),T(2,1),T(3,1),T(4,1),T(5,1),
6555 PRINT #5,T(6,1),T(7,1),T(8,1),T(9,1),T(10,1)
6560 PRINT #6,,k,,S,,T(1,2),T(2,2),T(3,2),T(4,2),T(5,2),
6565 PRINT #6,T(6,2),T(7,2),T(8,2),T(9,2),T(10,2)
6570 PRINT #7,,k,,S,,T(1,3),T(2,3),T(3,3),T(4,3),T(5,3),
6575 PRINT #7,T(6,3),T(7,3),T(8,3),T(9,3),T(10,3)
6580 PRINT #8,,k,,S,,T(1,5),T(2,5),T(3,5),T(4,5),T(5,5),
6585 PRINT #8,T(6,5),T(7,5),T(8,5),T(9,5),T(10,5)
6590 PRINT #9,,k,,S,,T(1,6),T(2,6),T(3,6),T(4,6),T(5,6),
6595 PRINT #9,T(6,6),T(7,6),T(8,6),T(9,6),T(10,6)
6600 print #10,,k,,s,,1/u(0,1),1/u(0,2),1/u(0,3),1/u(0,4),1/u(0,5),
6605 print #10,1/u(0,6),1/u(0,7),1/u(0,8),1/u(0,9),1/u(0,10)
6607 print #11,k,s,T(10,4),tps(0),ad
6608 print #11,hx,hy,hz,tv,tm
6610 PRINT "S=";S,"CC=";CC,"k=";k,"u=";u
6612 PRINT " TEMP(1)---TEMP(10)"
6614 PRINT T(1,5),T(2,5),T(3,5),T(4,5),T(5,5)

```

```

6616 PRINT T(6,5),T(7,5),T(8,5),T(9,5),T(10,5)
6620 PRINT "    TAU(1)---TAU(10)"
6622 PRINT T(1,1),T(2,1),T(3,1),T(4,1),T(5,1)
6625 PRINT T(6,1),T(7,1),T(8,1),T(9,1),T(10,1)
6630 PRINT "    P(1)---P(10)"
6640 PRINT P(1,0),P(2,0),P(3,0),P(4,0),P(5,0)
6645 PRINT P(6,0),P(7,0),P(8,0),P(9,0),P(10,0)
6650 PRINT "    Sy(1)---Sy(10)"
6660 PRINT S(1,0),S(2,0),S(3,0),S(4,0),S(5,0)
6665 PRINT S(6,0),S(7,0),S(8,0),S(9,0),S(10,0)
6670 PRINT "    ST(1)---ST(10)"
6680 PRINT T(1,4),T(2,4),T(3,4),T(4,4),T(5,4)
6685 PRINT T(6,4),T(7,4),T(8,4),T(9,4),T(10,4)
6690 PRINT "    D(1)---D(10)"
6700 PRINT 1/U(0,1),1/U(0,2),1/U(0,3),1/U(0,4),1/U(0,5)
6710 PRINT 1/U(0,6),1/U(0,7),1/U(0,8),1/U(0,9),1/U(0,10)
6720 PRINT "    Sx(1)---Sx(10)"
6760 PRINT T(1,6),T(2,6),T(3,6),T(4,6),T(5,6)
6765 PRINT T(6,6),T(7,6),T(8,6),T(9,6),T(10,6)
6770 PRINT "HX      HZ      TV      TM      AD"
6775 PRINT HX,HZ,TV,TM,AD
6790 PRINT
6800 RETURN

```

```

7000 REM  Subprogram for giving initial values

```

```

7200 DY=H/TI
7210 FOR X=1 TO TI
7220 H(X)=(2*X-1)*H/2/TI
7222 P(X,0)=P0
7224 TpS(X)=P0
7226 S(X,0)=0
7230 sw1=1
7235 gosub 2220
7250 NEXT X
7255 sw1=1
7260 FOR X=1 TO TI
7264 V(X,1)=P0
7266 V(X,2)=0.0001
7270 V(X,3)=0.0001
7278 F(X,1)=-1000
7280 F(X,2)=10

```

```

7282 F(X,3)=10
7300 if TT(X)>Tg(X) then 7320
7305 Vr(X)=Vso*(1-ar(X)*(T0-Tg(X)))*(1-ag(X)*(Tg(x)-TT(X)))
7310 U(0,X)=Vr(X)*(1-Kg0*P0)
7313 Vv(X)=Vso*(1-ag(X)*(T0-TT(X)))*(1-Kg0*P0)
7316 GOTO 7324
7320 Vr(X)=Vso*(1-ar(X)*(T0-TT(X)))
7322 U(0,X)=Vr(X)*(1-Ka0*P0)
7323 Vv(X)=Vso*(1-ag(X)*(T0-TT(X)))*(1-Ka0*P0)
7324 TA(X)=1-U(0,X)/Vv(X)
7326 TA(X)=abs(TA(X))
7328 Vs(X)=U(0,X)
7330 GV(X)=U(0,X)
7331 D1U(0,X)=0
7332 FG(X)=0
7333 VG(X)=VS(X)
7334 U(X,0)=U(0,X)
7337 GF(X)=0
7360 IF TT(X)>=TG(X) THEN 7385
7370 GF(X)=1
7375 FG(X)=1
7380 GOTO 7410
7385 FG(X)=0
7390 VG(X)=U(0,X)
7400 PG(X)=TpS(X)
7410 VE1=VR(X)*(1-AR(X)*(T0-TT(X)))
7420 VE2=VR(X)*(1-AR(X)*(T0-TG(X)))
7430 VE2=VE2*(1-AG(X)*(TG(X)-TT(X)))
7440 VE(X)=(1-FG(X))*VE1+FG(X)*VE2
7445 TAU(X)=TAU0*EXP(-BB*Kr0*abs(TpS(X)))
7455 TAU(X)=TAU(X)*EXP(-BF*(TA(X))^N(X))
7544 PF(X,0)=-1000
7546 S(X,0)=.0001
7548 VY(X)=0
7549 DVY(X)=0
7550 NEXT X

7555 FOR I=1 TO NF
7560 FOR Q=1 TO 4
7570 K(Q,I)=F(1,I)
7580 NEXT Q
7590 NEXT I

```

```

7600 FOR X=0 TO CN
7620 FOR Y=0 TO NL
7640 PF(X,Y)=0
7660 Q(X,Y)=0
7680 NEXT Y
7700 NEXT X
7710 for x=0 to Ti
7720 t(x,1)=tau(x)
7730 t(x,2)=Tag(x)
7740 t(x,3)=Nar(x)
7750 t(x,4)=P0
7760 t(x,5)=TT(X)
7770 t(x,6)=0.0001
7780 next x
7810 for x=1 to TI
7840 W(X)=U(0,x)
7860 U(x,0)=W(X)
7870 D1W(X)=0
7880 next x
7890 U(0,0)=W(1)
7900 Gosub 2000
7980 GOSUB 9710
7990 GOTO 580

```

8000 REM Subprogram for giving initial conditions and values

```

8010 H=.1
8020 T0=200
8025 TE=85
8040 OPT=.618
8050 IP=3.14159
8080 SV0=2.8
8085 Tv0=2*Sv0
8090 Vso=1.034
8095 Vs0=Vso
8100 V0=SV0/TI
8110 TTR=125
8120 TAU0=1.81*10(-8)
8130 TAG0=0.14676
8140 C3=.22
8150 Ag0=2.3*10(-4)
8160 Ar0=5.8*10(-4)

```

```
8170 Aa0=2.5*10^(-4)
8200 GG=1.5*10^9
8210 GR=2*10^5
8225 TG0=85
8250 S=1*10^(-9)
8255 sd=s
8260 DS=5*10^(-4)
8290 SV=0
8330 ATG=3.3*10^(-7)
8400 hy0=3.5
8410 hx0=8
8420 tv=2*sv0
8500 for x=1 to Ti
8510 TT(X)=T0
8520 next x
8600 CT1=-4.3
8610 CT2=80
8620 TRT=160
8888 GOTO 550
```

```
8910 FOR X=1 TO TI
8912 FOR Y=1 TO NF
8914 V(X,Y)=U(X,Y)
8916 NEXT Y
8918 NEXT X
8920 RETURN
```

```
9710 FOR X=1 TO TI
9720 FOR Y=1 TO NF
9730 U(X,Y)=V(X,Y)
9740 NEXT Y
9750 NEXT X
9760 RETURN
```

```
9900 REM End of the program
```

```
9910 CLOSE #1
9920 CLOSE #2
9930 CLOSE #3
9940 CLOSE #4
9950 CLOSE #5
9960 CLOSE #6
```

9970 CLOSE #7
9975 CLOSE #8
9980 CLOSE #9
9985 CLOSE #10
9990 CLOSE #11
9999 END

VITA

Xinhua (Sam) He was born in Fuzhou City, Fujian Province, China. The author attended elementary school in his hometown in 1961. Even though the Chinese authorities often disturbed the school system, to the point of shutting down all colleges and universities in the period 1966—1976 (the so-called "Cultural Revolution"), he managed a way to continue his studies. He graduated from high school in 1973. He completed the High Education Admission Test in 1977, which had not been given during the period 1966—1976. The author was admitted to the East China Institute of Textile Science and Technology (China Textile University) in the spring of 1978. He graduated with the degree of Bachelor of Science in Textile Engineering with the highest honors in 1982. He continued in the Textile Engineering at China Textile University and earned the Master of Science degree in 1984. Finally, he served as a lecturer at Fuzhou University from 1984 to 1989.

The author came to the United States and entered the graduate school of the University of Tennessee, Knoxville with a major in Polymer Engineering in the Department of Materials Science and Engineering in the spring of 1990. He received the Doctor of Philosophy degree in Polymer Engineering in August 1994.