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Mikael Rigdahl^a

^a Department of Polymeric Materials, Chalmers University of Technology, Sweden

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Calculation of Residual Thermal Stresses in Injection Molded Amorphous Polymers by the Finite Element Method

MIKAEL RIGDAHL

*Chalmers University of Technology
Department of Polymeric Materials, S-402 20 Gothenburg, Sweden*

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The finite element method (FEM) is used to calculate the distribution of residual internal stresses in an injection molded plate-shaped polystyrene specimen. The first step of the calculating procedure is the determination of the temperature distributions in the plate and its variation with cooling time. The temperature distribution data are then used for the determination of the corresponding stress distribution. Also this latter step is accomplished using the FEM-technique. The residual stress distribution is obtained when the sample has been cooled to the temperature of the mold. The main result of the calculations is the finding that the surface layer of the plate is subject to compressive stresses, while the interior accommodates stresses of tensile type. The calculations relate to a polystyrene specimen. The results are shown to agree well with earlier data concerning internal stresses in injection molded objects. The possible influence of anisotropy and visco-elastic relaxation has been neglected. The method can be applied to other amorphous polymers and, after a slight modification, also to polymers of semicrystalline type.

INTRODUCTION

Effects produced in injection molded parts by the combined action of anisotropy and residual thermal stresses are normally associated with the occurrence of "internal" or "frozen-in" stresses. Despite their obvious technical importance, the knowledge concerning the physical nature of these stresses, their measurement and influence on the properties of the molded part is highly limited. This applies also to the separation of the effects of anisotropy and true residual stresses.

The present paper is an account of a theoretical work the aim of which was to

calculate the magnitude of residual thermal stresses in an injection molded, rectangular (square) plate, where the possible role of anisotropy and thermal stress relaxation has been neglected. The mathematical technique employed is the numerical method of finite elements (FEM). The results obtained will be shown to agree qualitatively with previous data relating to thermal stress profiles measured by the thermal shrinkage method,¹ the method based on removing thin layers from the surface of the molding² and the measurement of hardness.³ The results also agree with previous calculations using somewhat less advanced mathematical tools.¹

The computer program based on the finite element method allows the calculation of the thermal stress profiles across the width of the sample at various times during cooling of the melt until the temperature of the solidifying melt and that of the mold have become equal. Another result is the variation of the sample temperature with time during the solidification of the melt. As the method cannot take account of relaxation effects, the results obtained give the theoretical maximum stresses not reduced by the action of viscoelasticity.

The difficulties in separating the contribution of anisotropy and thermal stresses in plastics seem to explain, at least partly, the limited amount of work published in this area. X-ray methods⁴ being a standard procedure in the metal field, cannot always be used with polymers, mainly because of their imperfect or even amorphous structure. A simple method, even though not easily amenable to physical interpretation, is the determination of thermal shrinkage.¹ For injection molded samples, this method usually shows the largest shrinkage near the surface; the shrinkage of the middle parts being substantially lower. Such stress profiles are normally discussed in terms of the temperature and pressure conditions prevailing during a molding cycle together with the changes in the morphology of the polymer.^{5,6} Using such a method, Knappe could show that negative thermal stresses amounting to 100–200 kp/cm² appeared in quenched polymeric samples. Their magnitude was dependent on the quenching conditions.¹

Another, rather crude method for studying thermal stresses is to successively remove thin layers of the polymer from the surface of the molding and to measure the resulting deformation.² Also hardness values have been used in order to calculate the internal stress level.³ This method gives directly a numerical value of the stress level. Measurements on polystyrene moldings showed negative stress values of ca. 100 kp/cm² near the surface. Finally one could mention the use of birefringence⁷ and holographic methods.⁸

For metals and ceramic materials, thermal stresses resulting from certain types of thermomechanical treatment have been calculated. Among the numerous examples, the thermal stress distribution in hot-rolled steel⁹ or in glass plate cooled from both sides^{10,11} can be mentioned. Both elastic⁹ and visco-elastic models^{10,11} were used in the calculations.

Theoretical calculations regarding polymers are far less numerous. Knappe¹ utilizing some results given by Timoshenko¹² considered a thin injection plate, neglecting relaxation effects. He arrived at the following formula giving the thermal stress distribution

$$\sigma_x = \alpha ET_0 \left(\frac{1}{3} - \frac{y^2}{c^2} \right) \quad (1)$$

where E is Young's modulus, α the thermal expansion coefficient, T_0 the difference between the temperature of the surface of the plate and the temperature at which the plate solidifies, σ_x the longitudinal stress in the plate, $2c$ the width of the plate and y is between $-c$ and c . According to Eq. (1), the stresses are highest at the surface ($y = \pm c$) of the molded part and they are negative (compressive stresses). This is in good agreement with the measurements mentioned *above*.¹ Further, this also justifies the elastic approach, neglecting relaxation effects, used in the calculations presented below.

GENERAL BACKGROUND

Thermal stresses in a solidifying polymer body are due to restraints occurring between parts of the body where the solidification process has reached different levels. In the initial stage, weak tensile stresses are present in the surface layers, primarily due to the weak constraint exerted by the molten interior. At the end of the process, a stress reversal has taken place, whereby large compressive stresses are produced at the surface, while the interior is in a state of tensile stress. It may be noted that no adhesion between the walls of the mold cavity and the polymer is necessary in order to explain the occurrence of such stress; they can appear in a freely solidifying body as well, provided the cooling is not slow enough.

The basic assumption in calculating thermal stresses in an element of a body being cooled under such constraints that thermal shrinkage is completely prevented is the following formula,

$$\sigma = E\alpha \Delta T \quad (2)$$

where σ is the stress developed during a temperature decrease ΔT , and E and α are the modulus of elasticity and the coefficient of thermal expansion, respectively. It is thus evident that a knowledge of the temperature distribution and its changes during cooling enables one to calculate the magnitude of the thermal stress in different parts of the body.

The temperature distribution is determined by the heat conduction equation together with appropriate boundary conditions,

$$\Delta T = C(T) \frac{\partial T}{\partial t} + Q(T) \quad (3)$$

where $C(T)$ is a temperature dependent quantity, $Q(T)$ the heat developed in the specimen and Δ the Laplacian.

The time dependent temperature differences between different parts of the body are transformed to equivalent temperature loads W , which in principle are given through an expression similar to Eq. (2). The deformation w in various parts of the body resulting from this load is

$$Bw = W \quad (4)$$

where B is a differential operator. If the body under study is a disc located in the xy -plane and the disc is assumed to be in a plane strain state, B has the form

$$B = - \frac{E(1-\nu)}{(1+\nu)(1-2\nu)} \begin{bmatrix} \frac{\partial^2}{\partial x^2} + \frac{1-2\nu}{2(1-\nu)} \frac{\partial^2}{\partial y^2} & \frac{1}{2(1-\nu)} \frac{\partial^2}{\partial x \partial y} \\ \frac{1}{2(1-\nu)} \frac{\partial^2}{\partial x \partial y} & \frac{\partial^2}{\partial y^2} + \frac{1-2\nu}{2(1-\nu)} \frac{\partial^2}{\partial x^2} \end{bmatrix}$$

where E is Young's modulus and ν Poisson's ratio for the material in question. The operator B is sometimes referred to as the structure stiffness.

Thus through Eq. (4) the time dependent deformation (w) in different parts of the body can be calculated. The corresponding transient thermal stress distribution is given from Hooke's law, which can be written as

$$\sigma = Hw \quad (5)$$

where σ corresponds to the stresses in the specimen and H is a matrix given by the theory of elasticity.

THE FINITE ELEMENT METHOD (FEM)

Equations giving the time dependent distributions of temperature, stress or strain in a molded specimen at various time during its cooling cannot, as a rule, be solved in closed form. Energy methods, often used in structural mechanics, have proved their usefulness in solving problems of this type. The finite element method used in the present case has the advantage that both the temperature and the stress distribution can be determined in an analogous way. The method of finite elements is an energy method, where the deformation of a body subjected to an arbitrary load is determined from minimum energy principles. In other words, one determines the deformation field resulting in a minimum potential energy of the system. The body under consideration is divided into a number of elements, preferably of a simple geometrical form. The corners of these elements are called nodes. When the body is subject to a load, the nodes are displaced. The aim of FEM is to calculate the displacement

field in a way which minimizes the potential energy of the system. The calculated field represents an approximation to the true state of the body, the deviation from this true state being dependent on the size of the elements.

As the FEM technique seems not to have been used previously for calculating thermal stresses in polymers, a short outline of the calculation of the stress distribution is given here. Calculating the temperature distribution is in all respects similar.¹³ The potential energy of a disc subjected to an arbitrarily distributed load, W , resulting in a deformation field, w , is given by the following expression.

$$F(w) = (w, Bw) - 2(w, W) \quad (6)$$

where (w, Bw) is the scalar product:

$$(w, Bw) = \int_{\Omega} Bw \cdot w \, d\Omega \quad (7)$$

and (w, W) is given as

$$(w, W) = \int_{\Omega} wW \, d\Omega \quad (8)$$

Ω is the area of the plate. It may be noted that $F(w)$ equals twice the potential energy.

From the variational calculus it is known that the deformation w that results from the load W gives the functional (6) its minimum value.

The plate is subdivided into a number of triangular elements. The points where the corners of the elements meet are called nodes.

The approximate solution to Eq. (4) is assumed to have the form

$$w_a(x, y) = \sum_{i=1}^r g_i(x, y) \cdot p_i \quad (9)$$

if the plate is placed in the x - y plane.

The functions $g_i(x, y)$, which are determined prior to the calculation, are the so-called coordinate functions and p_i represents the unknown (and sought) nodal displacements resulting from the load W . By variational methods it is possible to show that the deformation which minimizes the potential energy and thus is a solution to the differential equation $Bw = W$, can be obtained from

$$p = E^{-1}P \quad (10)$$

where P is a column matrix with r elements given as

$$p_i = (g_i, W) = \int_{\Omega} g_i(x, y)W(x, y) \, dx \, dy \quad (11)$$

where E is a symmetrical rxr stiffness matrix with the elements

$$E_{ik} = (g_i, Bg_k) = \int_{\Omega} g_i(x, y)Bg_k(x, y) \, dx \, dy \quad (12)$$

When the nodal displacements now have been determined, the stresses in each triangular element are given by Hooke's law.

If the disc is subject to a temperature change this change is transformed to an equivalent temperature load W_i (or temperature load vector P_i).

A general outline of the finite element method can be found in Ref.¹⁴

LIMITATIONS OF THE METHOD

The method of calculating thermal stresses as outlined above cannot take account of relaxation effects likely to occur during cooling of the sample. Thus the values obtained are maximum values constituting an upper boundary to the thermal stresses which can occur under given conditions of cooling a certain sample. Due to relaxation effects, the internal stresses actually occurring are lower. On the other hand, they will agree, with regard to their distribution, with the unrelaxed stresses. The same applies to the case of linearly visco-elastic bodies, whose relaxation leaves the thermal stress distribution unaffected, only causing an overall decrease of the stress values.^{10,11}

For polymers with a low relaxation rate at room temperature, such as PS and ABS, the error incurred due to relaxation effects appears to be relatively small and without practical significance.

In this investigation, the molded material is treated as being isotropic. This assumption seems justified here in view of the shape of the molding. There is on the other hand no difficulty in extending the analysis to anisotropic (orthotropic) bodies. Finally, it may be noted that the analysis has been restricted to a two-dimensional case, since the FEM-technique becomes difficult to handle when applied to three dimensions.

It may be added that the present calculations do not take account of any adhesion between the molding and the walls of the mold.

CALCULATIONS

Assumptions regarding specimen shape and material properties

The specimen analyzed here is shown in Figure 1. It is assumed to consist of normal polystyrene, having the physical characteristics given below. The injection molding conditions are assumed to be as follows: injection pressure 100 MPa, nozzle temperature 220°C, temperature of the mold 20°C.

The physical characteristics of the polystyrene used were assumed to vary with temperature in a linear manner or to remain constant. The following values were used.¹⁵

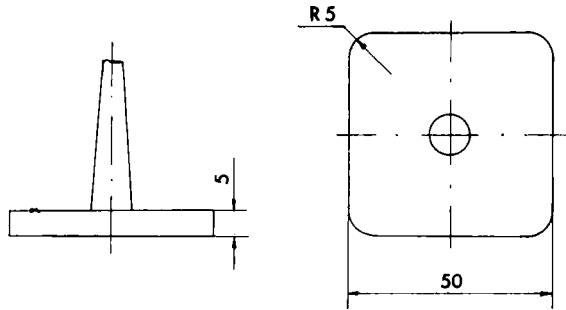


FIGURE 1 The geometry of the injection-molded sample. (All dimensions given in mm).

Specific heat

$$\begin{aligned} C_p(T)/C_p(298 \text{ K}) &= 0.105 + 0.029T & T < T_g \\ C_p(T)/C_p(298 \text{ K}) &= 0.64 + 0.021T & T > T_g \end{aligned}$$

Thermal conductivity

$$\begin{aligned} \lambda(T)/\lambda(T_g) &= 0.66 + 0.34T/T_g & T < T_g \\ \lambda(T)/\lambda(T_g) &= 1.20 - 0.20T/T_g & T > T_g \end{aligned}$$

Modulus of elasticity

$$\begin{aligned} E &= 3 \cdot 10^9 \text{ N/m}^2 & T < T_g \\ E &= 3 \cdot 10^5 \text{ N/m}^2 & T > T_g \end{aligned}$$

Coefficient of thermal expansion

$$\begin{aligned} \alpha &= 7 \cdot 10^{-5} \text{ K}^{-1} & T < T_g \\ \alpha &= 17 \cdot 10^{-5} \text{ K}^{-1} & T > T_g \end{aligned}$$

The density was set equal to 1050 kg/m^3 and independent of temperature. For the Poisson's ratio the value 0.32 was used below and 0.5 above T_g .

The influence of pressure on T_g was described by $dT_g/dp = 0.028 \text{ K/bar}$ in the 0–100 MPa range. The influence of pressure on the properties listed above e.g. C_p was obtained by shifting the C_p - T -curves parallel to the T -axis by the amount corresponding to the dT_g/dp -shift.¹⁶ All the other quantities were assumed independent of pressure. This was justified by results of considerations taking account of possible pressure effects.

To accomplish the continuous shifting of C_p and T_g with temperature and pressure an equation of state (p - v - T -relation) was needed. The Spencer-Gilmore equation¹⁷ was assumed valid for polystyrene in the molten state, i.e.

$$(p + \pi)(v - w) = R'T \quad (13)$$

with $\pi = 186,3 \text{ MPa}$, $w = 0,822 \cdot 10^{-3} \text{ m}^3/\text{kg}$ and $R' = 0.8 \cdot 10^{-4} \text{ MPa m}^3/\text{kg K}$. In Eq. (13) p denotes the pressure, v the specific volume and T the temperature.

Another property of importance in this connection is the surface conductance (α_s). The heat transfer at the surface (\dot{Q}) can be calculated as:

$$\dot{Q}_s = \alpha_s A (T_s - T_a) \quad (14)$$

where \dot{Q} = heat removed from the surface per unit time, α_s = surface conductance, T_s = temperature of the surface and T_a = temperature of the surroundings (in this case T_a is the mold temperature). The surface conductance can be split in three parts: conduction, convection, and radiation contributions. The convection contribution was neglected in this case. Similarly, the radiation was neglected, being at the highest temperature, at the most, 10% of the conduction and falling rapidly with decreasing temperature. In this case α_s was estimated to be 150 W/m² K.

Calculation of temperature and stress distributions in the specimen

We start by calculating the temperature distribution in the disc as a function of time. Suppose that the disc lies in the xy -plane and its thickness d in the direction of the z -axis is so small that the temperature can be taken as constant over it. Let α_s be the surface conductance of the material, λ its thermal conductivity, ρ its density and C_p its specific heat; then the differential equation the temperature should satisfy is:

$$\rho C_p(T) \frac{\partial T}{\partial t} = \lambda(T) \frac{\partial^2 T}{\partial x^2} + \lambda(T) \frac{\partial^2 T}{\partial y^2} - \frac{2\alpha_s}{d} (T - T_a) \quad (15)$$

where the specific heat and thermal conductivity are allowed to vary with temperature in the way described above. Eq. (15) is a special case of Eq. (3).

At the boundaries the cooling of the molded part is determined by the surface conductance in the following way

$$\lambda(T) \frac{\partial T}{\partial n} = \alpha_s (T_s - T_a) \quad (16)$$

where n is a vector normal to the surface of the part.

This boundary value problem was solved numerically using a FEM-based computer program developed for this purpose.

When the temperature distribution is calculated only one quadrant of the plate has to be considered. The plate is divided into triangular elements as shown in Figure 2 and the temperature is calculated in each node. The polymer is assumed to have a certain initial temperature relative to the mold (200 K). Two seconds after the cooling has started the temperature distribution is calculated. This calculation is repeated every two seconds for a period of 90 seconds.

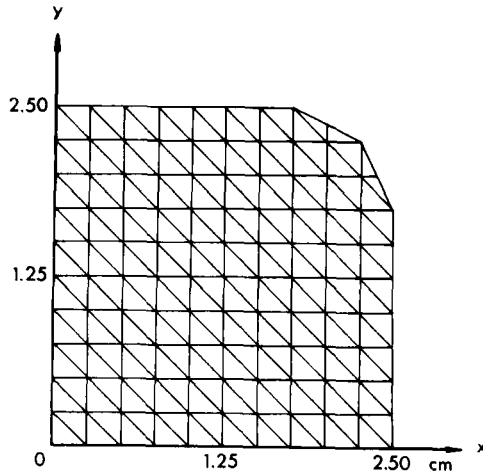


FIGURE 2 Element division of the first quadrant of the plate (118 nodes, 196 elements).

After each time step the temperature differences are transformed into equivalent temperature loads as described earlier. The corresponding deformation distribution w is then determined as a function of time by means of Eq. (4). When the deformation field is known the corresponding transient stresses are calculated using Hooke's law, Eq. (5).

A FEM-computer program has been developed for the elastic stress calculations. The same network can be used as in the temperature analysis (Figure 2). Using this method one obtains the thermal stress distribution built up in the disc as a function of time. When the part has attained the temperature of the mold, i.e. after a sufficiently long cooling time, the thermal stress values are those corresponding to the residual stress distribution. Since the disc can be assumed to have a constant thickness during solidification it seems plausible to consider a plane strain rather than a plane stress state as an appropriate description of the problem.

The two FEM-computer programs (temperature and stress distribution), are processed simultaneously by the computer.

RESULTS

In this section the time variation of the temperature distribution and the residual stresses in the part will be discussed.

The thermal analysis shows that the disc can be divided in two regions: (a) a narrow region near the walls of the mold that cools very rapidly and (b) the interior of the disc that cools at a substantially lower rate, Figure 3.

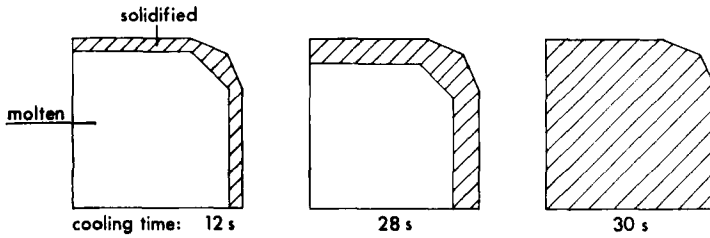


FIGURE 3 The solidification of the molded plate.

The cooling profiles for three different points are shown in Figure 4. The cooling rate is much faster for the points at the boundary than for the point in the middle and the difference between the two outer points is not very significant. As expected the passage through the glass transition point has no noticeable effect on the cooling profiles.

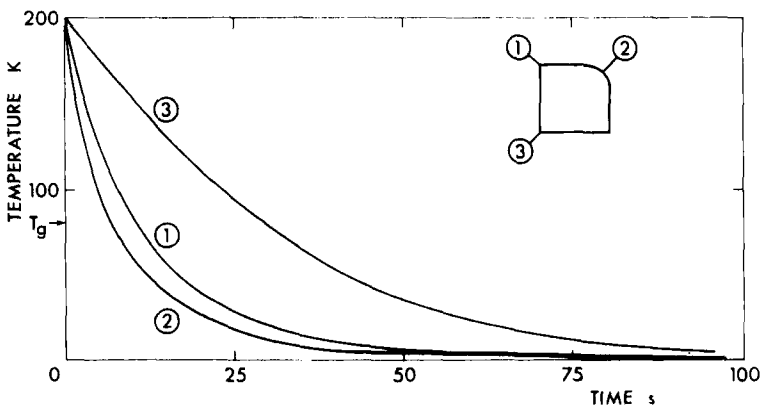


FIGURE 4 The cooling profiles for three different parts of the plate.

For semicrystalline polymers the corresponding cooling curves would exhibit a stepwise change in the slope in the solidification interval.

The development of thermal stresses is governed by temperature differences between different points of the plate within the temperature range in which solidification takes place, cf. Figure 5.

In Figure 5 the difference in temperature between point (1) and (3) is shown as function of time. The curve rises very sharply since the outer parts of the plate cool rapidly. The interval in which the plate becomes solid is indicated in the figure. This interval contains the greatest temperature difference (90°C) which has a strong influence on the magnitude of the residual stresses. At the end of the cooling stage the temperature difference goes to zero as expected.

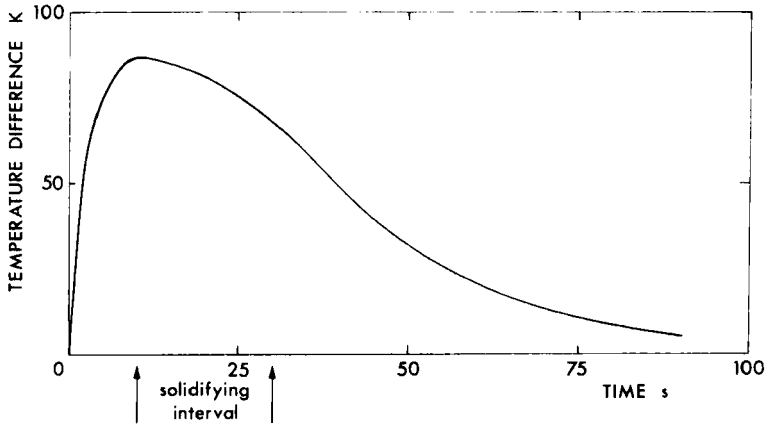


FIGURE 5 The temperature difference between point (1) and point (5) shown in Figure 4 as a function of time.

We now turn to the stress field. For symmetry reasons only the variation of the normal stress σ_x and the shear stress τ_{xy} is considered. Once again, at first only stresses in the areas around points (2) and (3) are discussed.

The stresses σ_x and τ_{xy} around point (2) are shown in Figure 6. During filling

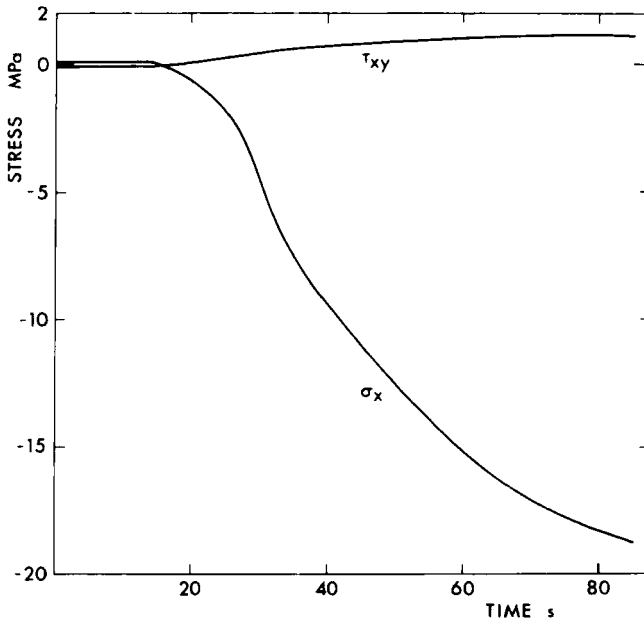


FIGURE 6 The normal (σ_x) and shear (τ_{xy}) stresses around point (2) shown in Figure 4 as a function of time.

of the mold the outer parts of the plate, i.e. those in contact with the walls of the mold cavity, are cooled at a high rate.

Being prevented from free shrinkage, these parts accommodate small tensile stresses. For stress balance reasons, the interior of the plate contains corresponding compressive stresses. The result of the calculations relating to the normal stress σ_x shown in Figure 6 confirm this picture, σ_x having small positive values for cooling times up to 15 s (a somewhat clearer picture of this stress is given in Figure 8). After some time, the temperature in the interior of the plate has decreased. Free shrinkage of the interior is now prevented by the stiffness of the surface layers which have solidified earlier.

The result of this is that the stresses in the surface layer turn negative (compressive stresses) while the interior of the plate now contains tensile stresses (see also Figure 9). The magnitude of the negative stress in the surface layers is considerable, Figure 6. The shear stresses, on the other hand, are negative in the beginning of the cooling process and positive at the end of it. The maximum value of τ_{xy} is only about a tenth of the normal stress σ_x .

Figure 7 shows the stress σ_x in the middle of the plate. The time dependence of the stress is in accordance with what has been said above. At first the stress is negative for 26 s in the rubbery state, whereafter it assumes a comparatively

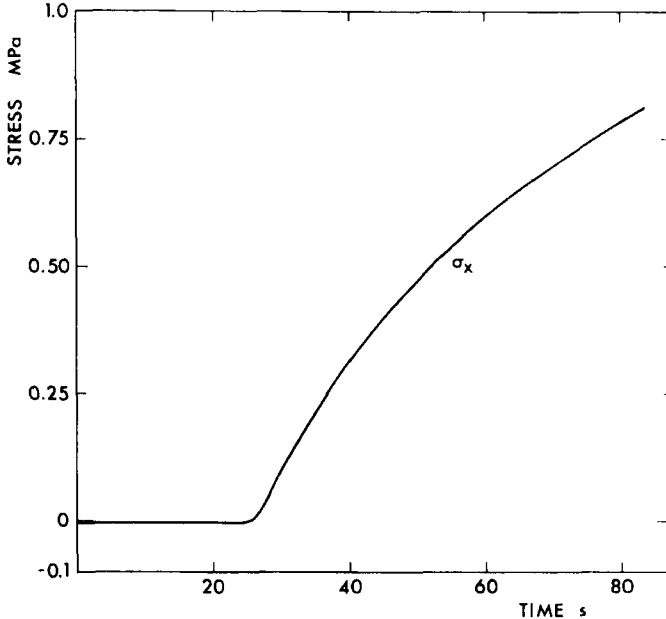


FIGURE 7 The normal stress (σ_x) in the middle of the plate as a function of time.

large positive value. This change occurs, as expected, later than the corresponding change for those parts of the plate lying near the cavity walls. The residual stress level is far lower ($\sim 1/10$) that the residual stress value near the cavity walls. For symmetry reasons the shear stress τ_{xy} is zero in the middle of the plate.

In Figures 8 and 9 the normal stress distribution σ_x is shown along the x -axis at the beginning and end of the cooling process respectively. In the initial stage the stresses are positive at the boundary and negative in the interior of the plate; they are comparatively small. When the cooling has ended the situation is altered. The surface stresses then become negative, while the interior accommodates tensile stresses. The magnitude of these thermal residual stresses is much larger than that of the stresses at the beginning of the cooling process.

The normal stresses σ_y and σ_z show a dependence on time and position which is similar to σ_x .

This change with time from positive to negative stresses and vice versa is in agreement with similar results concerning stresses in hot-rolled steel beams.⁹

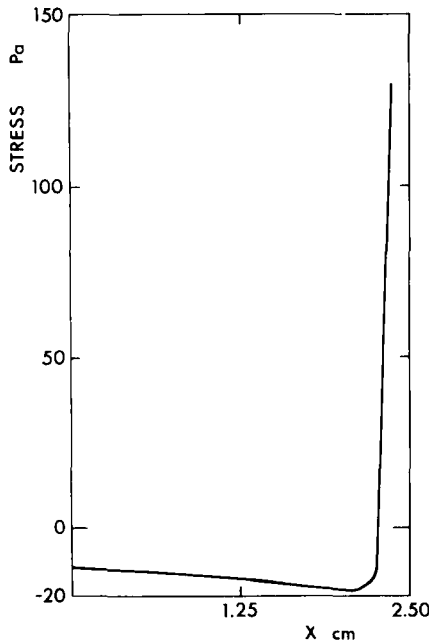


FIGURE 8 The normal stress distribution (σ_x) along the x -axis (shown in Figure 2) after 2 s.

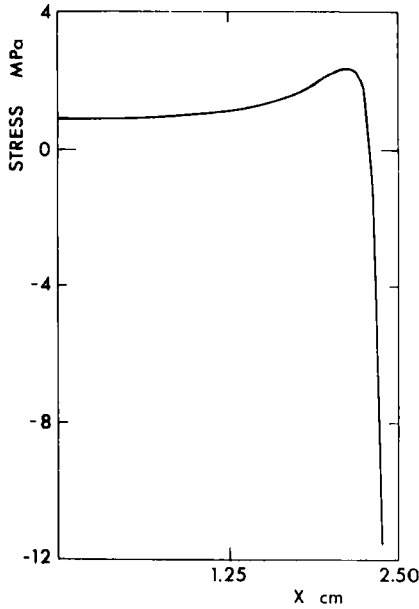


FIGURE 9 The residual stress distribution (σ_x) along the x -axis.

FINAL REMARKS

The results obtained seem to agree well with the general thermal stress pattern observed earlier on steel beams⁹ and glasses.^{10,11} Considering what has been said above about the origin of such stresses this is hardly surprising. In fact, thermal stress patterns of the type found here should be common to all solidifying bodies having a non-homogeneous temperature distribution. In all such cases, the solidified outer layers provide the initial constraint, which may or may not be accentuated by possible adhesion effects.

The FEM-computer programs used are quite general and easily adaptable to handle additional boundary conditions, like a varying amount of adhesion between the solidifying body and its surroundings. Also the effect of time, that is the effect of the relaxation likely to be encountered in certain polymeric systems, could be taken into account. The fact that our results agree with earlier calculations and experimental findings shows, that the relaxation effects are comparatively small and that the procedure can be applied directly without further corrections for possible time effects. With softer polymers, like polyethylene, the situation may, however, be different, as relaxation effects in such a polymer are known to occur at a substantial rate at moderate temperatures. One of the features of the FEM-programs used is its ability to calculate

the thermal stress distribution at various times during the cooling procedure. The thermal stress reversal, both in the surface layers and in the interior of the body are clearly brought out in this way.

Needless to say, the method can be applied to any polymer whose physical characteristics relevant in the present context are known. Such properties include for instance the effect of pressure and temperature on the T_g - and T_m -values. There are, for instance, no physical difficulties involved in including crystalline polymers in this treatment.

A short remark, finally, may be devoted to the possible influence of the injection pressure. As well known, such pressures are comparatively high, of the order of magnitude 50–100 MPa. In the present case, no account has been taken of such effects, simple considerations having demonstrated that the influence of the injection pressure of normal magnitude (≤ 100 MPa) on the thermal stress distribution is of minor importance only.

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