

Thermo-Viscoelastic Model for Shrinkage and Warpage Prediction During Cooling and Solidification of Automotive Blow Molded Parts

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ABSTRACT

Blow moulding is one of the most important polymer processing methods for producing complex thermoplastic automotive parts. Contrary to injection molding, little attention has focused on process control and simulation of blow molding processes. Yet, there are still several problems that affect the overall success of forming these parts. Among them are thermally induced stresses, relevant shrinkage and part warpage deformations caused by inappropriate mold design and/or processing conditions. Tolerance issues are critical in automotive applications and therefore part deformation due to solidification needs to be controlled and optimized accordingly. The accurate prediction tool of part deformation due to solidification, under different cooling conditions in automotive formed parts, is important and highly suited for part designers to help achieve an efficient production.

This paper describes in detail the three dimensional membrane element in large displacement formulation with an integration and implementation of the KBKZ constitutive equation to model the blowing phase of forming processes. Thereafter, we focus on the development of a linear thermo-viscoelastic constitutive equation based on a Zener model for modeling shrinkage and warpage of molten-solidified polymeric material during the cooling and solidification. The derivation of the governing equations as well as the implementation in our BlowView software is discussed and presented. The finite element method (FEM) will be used to numerically solve the derived governing equations and the shell theory, presented as an assemblage of flat elements formed by combining the Constant Strain Triangle element (CST) and Discrete Kirchhoff plate theory (DKT element), is applied. This shell theory is well suited for thin complex blow molded automotive parts. The numerical implementation and integration in BlowView is presented in detail.

Finally, finite element warpage simulation results in terms of displacements and deformations, obtained with this formulation are presented for a simple and complex automotive part. The simulation results are compared to experimental and literature results to determine the accuracy and the limitations of the proposed model.

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INTRODUCTION

The thermoplastic forming processes are those where a molten polymeric parison and/or sheet is deformed to take the shape of a mould cavity and subsequently solidifies. Since they are highly automated processes, they are predestined for large-scale manufacturing. The thermoplastic forming market

is expanding to more complex geometries and a larger list of potential materials. Therefore, part designers in today's global environment are under increasing pressure to reduce part development time to a minimum, yet ensuring the maximum part quality and minimum manufacturing costs. Nowadays, part designers pay increasing attention to part warpage, which becomes a determining quality criterion for part acceptance.

especially for automotive applications where tolerance issues are so critical. Therefore, the accurate prediction of part deformation due to solidification in automotive parts is an important aspect to be addressed and controlled in order to achieve an efficient production [1].

During these processes, the so called process-induced residual stresses are caused by differential shrinkage, which, in turn, is caused by inhomogeneous in-molding cooling and solidification of the thermoplastic material. These internal stresses act on the part with effects similar to externally applied forces, and they are the forces that drive post-ejection part warpage. In thermoplastic forming industry, it is well known that the magnitude of the induced residual stresses depend on the processing conditions (polymer temperature, mould temperature, cooling time, and part thickness distribution), mold design and part specifications. The out-mold relaxation of these stresses cause the part to deform in order to reach an equilibrium state. The equilibrium state means that there is no external force exerting on the part and the tensile and compressive stresses over part cross-section should balance with each other [2]. On the other hand, if the stresses are not allowed to relax, via excessive in-mould cooling or a fixation device, mechanical failure can occur.

Since tolerance and part failure issues during forming operation are critical in many applications, particularly in the automotive industry, the part deformation due to the cooling and solidification needs to be controlled and optimized accordingly. Therefore, it is important for the designer to achieve an optimal balance between the level of deformation and the amount of residual stresses. Modeling of the deformation and residual stresses allows the designer to obtain this balance off-line, with minimal experimental trials [3]. Furthermore, if the polymeric behavior can be modeled adequately in a simulation, two major advantages can be achieved: first, the influence of different processing variables on the non-uniform differential shrinkage can be investigated and consequently adjusted and controlled in a way to minimize final residual stresses; second, the knowledge of residual stresses allows the prediction warpage behavior of a product. If the dimensional changes of a part can be estimated before a tool is built, the design engineer gets a valuable tool to avoid costly and expensive modifications to the mould [4].

In this article, a numerical model for the prediction of thermally induced stresses as well as resulting shrinkage and warpage during solidification is studied using BlowView¹. First, the thermal model used for computing the temperature field of formed parts taking into account polymer crystallization is presented. Thereafter we examine the formulation and the integration of the K-BKZ constitutive equation to model the blowing phase of the forming processes. Finally, a special emphasis is placed on the Zener model and its recurrent formulae used for incremental

calculation of time-dependent residual stresses. The warpage deformation of the part based on a thermo-viscoelastic model is finally derived for small strains formulation under small displacement theory.

THEORETICAL APPROACH

Thermal Model

To evaluate the thermally induced residual stresses developed during the blowing and stretching stages as well as the cooling and solidification stages, both inside the mould and after demoulding, a good prediction of the temperature field evolution is first required. Given the inherent low thermal conductivity of plastics, the special geometrical configuration of the formed part i.e. relatively thin compared with their surface area, unilateral cooling is usually assumed to be a one dimensional transient heat conduction problem through the part thickness [4, 5]. Taking into account the effect of heat absorption due to crystallization of the polymer during the cooling stage leads to the following heat balance equation [4]:

$$\rho C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x} \right) + \dot{Q}_{cry} \quad (1)$$

where ρ , C_p and k are the density, specific heat and thermal conductivity of the polymer respectively that may be considered constant or temperature dependent [3, 4], T is the temperature and t is the elapsed time. The $\dot{Q}_{cry}$ term describes the volumetric heat absorption due to crystallization.

The solution of the balance energy equation (1) depends on the initial temperature values and on the boundary conditions. As initial conditions for the cooling stage, we use the final temperature field provided at the end of the forming stage. It is then assumed that the energy interchange between the outer surface of the part and the surface of the mould before demoulding, and surrounding air after demoulding, occurs by free convection. The energy interchange between the inner surface and cavity air also occurs by lateral free convection. The boundary conditions on the inner and outer surface of the part before demoulding and after demoulding are given as follows:

$$-k \frac{\partial T}{\partial x} = h_{air}^{part} \cdot (T_s^{in} - T_{air}^{in}) \quad (2)$$

$$-k \frac{\partial T}{\partial x} = h_{mould}^{part} \cdot (T_s^{out} - T_{mould}) \quad (3)$$

¹BlowView is an engineering simulation software developed at NRC-Automotive that can handle extrusion blow molding, injection blow molding, stretch blow molding and thermoforming [1, 2, 3, 4].

$$-k \frac{\partial T}{\partial x} = h_{air}^{Part} \cdot (T_s^{in} - T_{air}^{in}) \quad (4)$$

$$-k \frac{\partial T}{\partial x} = h_{air}^{Part} \cdot (T_s^{out} - T_{air}^{out}) \quad (5)$$

where h_{air}^{Part} and h_{mould}^{Part} are the convection coefficients between the surface of the part and the air, and the surface of the part and the mould, respectively. They may be considered constant or, more realistically, variable with time and position [2]. T_s^{in} and T_s^{out} are the inner and outer surface temperature of the part, respectively. T_{air}^{in} and T_{air}^{out} are the inner and the outer air temperature and T_{mould} is the mould temperature.

In equation (1), the crystallization heat absorption $\dot{Q}_{cry}$ term is given by the following equation:

$$\dot{Q}_{Cry} = (\rho \Delta H_{Cry}) \cdot \frac{\partial \chi}{\partial t} \quad (6)$$

where ΔH_{cry} is the latent heat of crystallization and χ is the relative degree of crystallinity. According to [6, 7, 8], the Nakamura model is a well-known model for the prediction of crystallinity during polymer processing. The model is a differential expression that gives the rate of crystallization $\frac{\partial \chi}{\partial t}$ as a function of the temperature T:

$$\frac{\partial \chi}{\partial t} = nK(T)(1 - \chi) \cdot \left[\ln \left(\frac{1}{1 - \chi} \right) \right]^{\left(\frac{n-1}{n} \right)} \quad (7)$$

Where n is the Avrami exponent and $K(T)$ is the temperature dependent rate constant parameter given by the Hoffman-Lauritzen theory through the following expression:

$$K(T) = K_0 \exp \left(\frac{U}{R(T - T_g + 30)} \right) - \frac{C(T + T_m)}{2T^2(T_m - T)} \quad (8)$$

where K_0 is the model constant, U the activation energy, R is the universal gas constant, C is the nucleation exponent, T_g is the glass transition temperature and T_m is the melting temperature.

The set of partial differential equations (1), (2), (3), (4), (5) describing such a problem is often referred to as the mathematical form or strong form. The differential equations may be either linear or non linear. Consequently, the exact analytical solutions of the heat transfer governing equations can only be obtained for problems in which restrictive simplifying assumptions are made with respect to geometry, material properties and boundary conditions. There is therefore, no option but to turn to numerical solution methods for the analysis of practical problems, where such simplifications are generally not possible.

Thermal finite element discretization

Based on the Galerkin approximation method and combining the balance equation (1) and the boundary conditions (2), (3), (4), (5) it is simple to show that the previous thermal problem is reduced to the following compact matrix form [9]:

$$[C(T)]\{\dot{T}\} + [K(T)]\{T\} = \{F(T)\} \quad (9)$$

in which,

$$\{T\} = \{T_n\}$$

$$C_{ij} = \int_{\Omega} (N_i \cdot \rho C_p(T) \cdot N_j) d\Omega$$

$$K_{ij} = \int_{\Omega} \left(\frac{\partial N_i}{\partial x} k(T) \cdot \frac{\partial N_j}{\partial x} \right) d\Omega + \int_{\Gamma_{Mold}} (N_i \cdot h_{Mold}^{Part} \cdot N_j) d\Gamma + \int_{\Gamma_{in}} (N_i \cdot h_{air}^{Part} \cdot N_j) d\Gamma + \int_{\Gamma_{out}} (N_i \cdot h_{air}^{Part} \cdot N_j) d\Gamma$$

$$F_i = \int_{\Omega} \left(N_i \cdot \rho \Delta H_{Cry} \cdot \frac{\partial \chi}{\partial t} \right) d\Omega + \int_{\Gamma_{Mold}} (N_i \cdot h_{Mold}^{Part} \cdot T_{Mold}) d\Gamma + \int_{\Gamma_{in}} (N_i \cdot h_{Mold}^{Part} \cdot T_{air}^{in}) d\Gamma + \int_{\Gamma_{out}} (N_i \cdot h_{air}^{Part} \cdot T_{air}^{out}) d\Gamma$$

Where, the component of vector T_n are the nodal temperatures and N_i are the element shape functions. For the transient case under consideration, the global capacitance $[C]$ and conductance matrices $[K]$ are temperature dependent. The non-linearity is due to the temperature dependent thermal conductivity, density, specific heat, and non-isothermal crystallization kinetics. Since $[C]$, $[K]$, and $\{F\}$ may strongly depend on the unknown temperature, the system of equations (9) may be strongly nonlinear. Also, Ω is the initial volume of the deformable thermoplastic continuous body (parison and/or sheet) and Γ is the surface boundary of this volume. Γ_{in} and Γ_{out} are respectively, the inner side and the outer side of the surface Γ , that are in contact with air. Γ_{Mold} is the part surface that is in contact with the mold.

Resolution strategy

The numerical solution of equation (9) is obtained by replacing the differential equations with finite difference relationships. Generally, a two-level time scheme is applied, where the solution at a particular time level is directly calculated from the temperature at a previous time level. The following relation is obtained [7]:

$$[C(T_{t+\tau\Delta t})]\left\{\frac{T_{t+\Delta t} - T_t}{\Delta t}\right\} + [K(T_{t+\tau\Delta t})]\{T_{t+\Delta t}\} = \{F(T_{t+\Delta t})\} \quad (10)$$

Using this algorithm with $\tau = 0$ corresponds to the Explicit Euler Scheme. The discrete set of differential equations becomes:

$$[C(T_t)]\{T_{t+\Delta t}\} = [[C(T_t)] - \Delta t[K(T_t)]]\{T_t\} + \Delta t\{F(T_t)\} \quad (11)$$

Where the resolution at time $t + \Delta t$ requires the inversion of the capacitance matrix $[C]$. It can be seen from [equation \(11\)](#) that the temperature value at time $t + \Delta t$, $T_{t+\Delta t}$, is directly evaluated from the current values at time t , T_t thereby returning the explicit nature of the algorithm. It was proved that this algorithm is conditionally stable and of first order of accuracy. According to the level of non-linearity this scheme seems well adapted to our problem with relatively small time increment of Δt ; [9].

Forming Deformations Model

In thermoplastic forming processes, the initial deformable thermoplastic body is geometrically completely defined. Therefore, a total Lagrangian formulation with the reference configuration as the initial undeformed configuration is adopted. Since most of the final products in thermoplastic forming processes consist of thin walled structures, in this paper we assume that the thermoplastic material is modeled as a three-dimensional thin membrane structure [5]. Each material point $\mathbf{P}$, belonging to the body Ω bounded by Γ , can be identified by two curvilinear coordinates (ξ, η) defined on the membrane mid surface, which remain constant at the time of forming. Consequently, the position of the point $\mathbf{P}$ belonging to this mid surface will be defined, in the undeformed reference configuration, by the vector $\mathbf{X}(\xi, \eta)$ and, in deformed configuration, by the vector, $\mathbf{x}(\xi, \eta)$. At the mid-surface point $\mathbf{P}$, a local tangent vectors are defined for undeformed and deformed configuration from the following classical formulas, respectively [10]:

$$t_g^1 = \frac{\partial \mathbf{X}}{\partial \xi}; t_g^2 = \frac{\partial \mathbf{X}}{\partial \eta} \quad (12)$$

$$t_g^1 = \frac{\partial \mathbf{x}}{\partial \xi}; t_g^2 = \frac{\partial \mathbf{x}}{\partial \eta} \quad (13)$$

We define $\vec{n}$ as the outward unit vector normal to the tangent plane at point $\mathbf{P}$ on the deformed boundary surface $\Gamma_p \in \Gamma$ defined from [\(12\)](#) as:

$$\vec{n} = t_g^3 = \frac{\frac{\partial \mathbf{x}}{\partial \xi} \times \frac{\partial \mathbf{x}}{\partial \eta}}{\left\| \frac{\partial \mathbf{x}}{\partial \xi} \times \frac{\partial \mathbf{x}}{\partial \eta} \right\|} \quad (14)$$

Although we are dealing with membrane model in this paper, a 3D variational formulation of the forming model is presented in this section. Based on the principal of stationary potential energy, we know that the total energy Π of a deformable body submitted to external loads tends to a minimum with regards to the displacement, which is expressed as [10]:

$$\delta \Pi = \delta \Pi_{\text{int}} - \delta w_{\text{ext}} = 0 \quad (15)$$

Where $\delta \Pi_{\text{int}}$ is the variation of strain energy of the deformable body and δw_{ext} is the variation of the work of external forces, which is given by the following expression:

$$\delta w_{\text{ext}} = \int_{\Omega} \delta \mathbf{u}^T \cdot \mathbf{f}_v d\Omega + \int_{\Gamma} \delta \mathbf{u}^T \cdot \mathbf{f}_s d\Gamma \quad (16)$$

Where $\mathbf{f}_v$ is body volume force vector and $\mathbf{f}_s$ is external surface force vector. $\delta \mathbf{u}^T$ is the transposed virtual displacement vector, that is compatible with displacement boundary conditions.

The variation of the work due to the volume forces is constant and usually neglected near to the external surface force. In thermoplastic forming processes the external surface force is due to the applied blowing pressure p , and therefore the variation of the work of external forces is reduced to the following form:

$$\delta w_{\text{ext}} = \int_{\Gamma_p} (p - p_a) \delta \mathbf{u}^T \cdot \vec{n} d\Gamma \quad (17)$$

The incremental form of [\(15\)](#) is given as follows:

$$\Delta \delta w_{\text{ext}} = \int_{\Gamma_p} (p - p_a) \delta \mathbf{u}^T \cdot \left(\frac{\partial \vec{n}}{\partial \mathbf{u}} \right) \Delta \mathbf{u} d\Gamma \quad (18)$$

The pressure p is assumed independent from the displacement in this study. In Lagrangian formulation, the variation of the strain energy can be expressed as a function of the 2nd Piola-Kirchoff stress tensor $\mathbf{S}$ and the conjugated Green-Lagrange strain tensor $\mathbf{E}$ as follows:

$$\delta \Pi_{\text{int}} = \int_{\Omega} \text{tr}(\delta \mathbf{E}^T \cdot \mathbf{S}) d\Omega \quad (19)$$

$$\mathbf{E} = \begin{bmatrix} E_{XX} & E_{XY} & E_{XZ} \\ E_{XY} & E_{YY} & E_{YZ} \\ E_{XZ} & E_{YZ} & E_{ZZ} \end{bmatrix} \text{ and } \mathbf{S} = \begin{bmatrix} S_{XX} & S_{XY} & S_{XZ} \\ S_{XY} & S_{YY} & S_{YZ} \\ S_{XZ} & S_{YZ} & S_{ZZ} \end{bmatrix} \quad (20)$$

Where Ω is initial volume of the deformable thermoplastic body. Relative to the reference configuration, the Green-Lagrange strain tensor is given by the following matrix form:

$$E = \frac{1}{2} [F^T F - I] \quad (21)$$

Where F is the material deformation gradient tensor defined from the displacement field $U(X, t)$ generated by the movement of the point P . A displacement field is a vector field of all displacement vectors for all particles in the body, which relates the deformed configuration with undeformed configuration. The displacement is expressed in terms of material coordinates as:

$$\mathbf{u}(\mathbf{X}, t) = \mathbf{x}(\mathbf{X}, t) - \mathbf{X} \equiv \begin{Bmatrix} u(\mathbf{X}, t) \\ v(\mathbf{X}, t) \\ w(\mathbf{X}, t) \end{Bmatrix} = \begin{Bmatrix} x(\mathbf{X}, t) \\ y(\mathbf{X}, t) \\ z(\mathbf{X}, t) \end{Bmatrix} - \begin{Bmatrix} X \\ Y \\ Z \end{Bmatrix} \quad (22)$$

With X been the position of point P in the undeformed configuration and x the position of the same point in the deformed configuration. The material deformation gradient tensor is then defined as:

$$F(\mathbf{X}, t) = \frac{\partial \mathbf{x}(\mathbf{X}, t)}{\partial \mathbf{X}} = \begin{bmatrix} \frac{\partial x}{\partial X} & \frac{\partial x}{\partial Y} & \frac{\partial x}{\partial Z} \\ \frac{\partial y}{\partial X} & \frac{\partial y}{\partial Y} & \frac{\partial y}{\partial Z} \\ \frac{\partial z}{\partial X} & \frac{\partial z}{\partial Y} & \frac{\partial z}{\partial Z} \end{bmatrix} \quad (23)$$

The virtual Green-Lagrange strain tensor is given by the following matrix form:

$$\delta E = \frac{1}{2} [\delta F^T F + F^T \delta F] \text{ and } \delta F = \left[\frac{\partial (\delta \mathbf{u}(\mathbf{X}, t))}{\partial \mathbf{X}} \right] \quad (24)$$

Therefore, the variation of the strain energy (19) can be expressed as:

$$\delta \Pi_{\text{int}} = \int_{\Omega} \text{tr} \left(\frac{1}{2} [\delta F^T F + F^T \delta F]^T . S \right) d\Omega \quad (25)$$

By using the vector expression of tensor δE^T and S , [equation \(25\)](#) is rewritten under the following form:

$$\delta \Pi_{\text{int}} = \int_{\Omega} \delta E^T . S d\Omega \quad (26)$$

The incremental form of [\(26\)](#) is given as follows:

$$\Delta \delta \Pi_{\text{int}} = \int_{\Omega} \Delta \delta E^T . S d\Omega + \int_{\Omega} \delta E^T . \Delta S d\Omega \quad (27)$$

The first term of [equation \(27\)](#) could be rewritten by using the vector form of the material deformation gradient tensor:

$$\int_{\Omega} \Delta \delta E^T . S d\Omega = \int_{\Omega} \delta F^T . \bar{S} . \Delta F d\Omega \quad (28)$$

$\bar{S}$ is known as the exploded form of the Piola-Kirchoff stress tensor and defined as:

$$\bar{S} = \begin{bmatrix} S & 0 & 0 \\ 0 & S & 0 \\ 0 & 0 & S \end{bmatrix}_{(9 \times 9)} \quad (29)$$

The matrix expression S is given by [equation \(20\)](#).

The second term of [equation \(27\)](#) could be rewritten in the following manner:

$$\int_{\Omega} \delta E^T . \Delta S d\Omega = \int_{\Omega} \delta E^T . \left(\frac{\partial S}{\partial E} \right) . \Delta E d\Omega \quad (30)$$

Therefore the incremental form of [equation \(26\)](#) could be presented as follows:

$$\int_{\Omega} \delta F^T . \bar{S} . \Delta F d\Omega + \int_{\Omega} \delta E^T . \left(\frac{\partial S}{\partial E} \right) . \Delta E d\Omega \quad (31)$$

Using Taylor series development formulae, the incremental form of [equation \(15\)](#) is given as follows:

$$\delta \Pi_{\text{int}} + \Delta(\delta \Pi_{\text{int}}) - (\delta w_{\text{ext}} + \Delta(\delta w_{\text{ext}})) \approx 0 \quad (32)$$

All members of the previous equation are defined by [equations \(17\), \(18\), \(26\) and \(31\)](#).

$$\begin{aligned} & - \int_{\Gamma_p} (p - p_a) \delta \mathbf{u}^T . \vec{n} d\Gamma - \int_{\Omega} \delta \mathbf{u}^T . f_v d\Omega \\ & - \int_{\Gamma_p} (p - p_a) \delta \mathbf{u}^T . \left(\frac{\partial \vec{n}}{\partial \mathbf{u}} \right) \Delta \mathbf{u} d\Gamma \\ & + \int_{\Omega} \delta E^T . S d\Omega \\ & + \int_{\Omega} \delta F^T . \bar{S} . \Delta F d\Omega \\ & + \int_{\Omega} \delta E^T . \left(\frac{\partial S}{\partial E} \right) . \Delta E d\Omega \approx 0 \end{aligned} \quad (33)$$

Finite element space discretization of the forming model

The finite element method is used to perform the space discretization of the incremental stationary potential energy [equation \(33\)](#). The initial deformable thermoplastic body is subdivided into three node isoperimetric triangular finite element. The element shape functions N_1 , N_2 and N_3 for the reference element are given as follow [\[11\]](#):