Software package and mathematical models of polymeric material heating and forming for quality analysis and control of multi-assortment hollow volume products

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Abstract. We have developed a software package which uses mathematical models of the key stages of polymeric material thermoforming in order to solve quality analysis and control problems for axisymmetric hollow volume products. Those types of products are commonly used for packaging and vary in their configurations and geometric parameters. The software package includes modules for calculating state parameter fields for polymeric material at different stages of heating and forming, a module for calculating product quality indices, databases containing information about polymers, forming tools, and permitted control action ranges, modules for visualization of modeling results in form of 2D and 3D graphs of state parameter distributions, as well as visualizing 3D models of prepared material and product with coloring. The software package can be configured for various types of polymers and products. The package’s core consists of a library of configurable mathematical models. It includes models describing two-sided radiant (one and multi zone) heating polymeric materials, biaxial stretching of polymeric materials during mechanical forming, and diffusive permeability of penetrants of various types (water vapor, oxygen) through product walls. The package serves as an effective tool for supporting production personnel in analyzing cause-effect relationships for the control object, and determining control actions at key stages of thermoforming that ensure quality requirements (thickness, equal thickness, barrier characteristics) are met when dealing with multi-assortment products made of polymeric films and sheets.

1. Introduction
Thermoforming is one of the main methods for producing hollow volume products from polymeric materials (films, sheets) which are used, in part, as packaging materials. It consists of:

- heating the prepared material to the temperature at which the polymer is most deformable during stretching without becoming damaged, resulting from macromolecule segment mobility;
- forming the heated material into the required product via a pressure differential above and below the material [1].

Thermoforming enables production of thin products of various configurations. The simplicity of producing the forming tools (matrices, punches) and their relatively low cost ensures low production
costs for the packages, whether at high or low volume. This is particularly important in markets with strong, constant competition. Production competitiveness can also be supported by meeting certain quality indices. Packaging material quality shows itself by ensuring the packaged good’s safety from the exterior environment for the guaranteed period.

The strictest requirements on packaging materials’ quality indices are placed on packaging materials for pharmaceutical products and foodstuffs, particularly their barrier properties (impermeability to water vapor and oxygen) and durability. These characteristics aren’t just dependent on the type of polymer, the thickness distribution (thickness variation) of the packaging also plays a major role. Should a section of the packaging be thinner than its neighboring regions, it would be more permeable to water vapor and oxygen, and would be less durable. Heightened water vapor permeability leads to pills partially dissolving. Heightened oxygen permeability leads to food product oxidation. Lower durability shows itself when packaging breaks down due to some external stress prior to the guaranteed date. It is important to implement heating and forming modes that enable the required thickness distribution. This guarantees that the produced packaging has the necessary barrier properties and durability to meet customer requirements defined by the packaging use case. The most promising approach to achieve this thickness distribution is to set an uneven temperature distribution along the surface of the prepared material at the beginning of the forming stage [2]. The goal is to make it so that the most deformable regions of the formed material (the thinnest regions of the product) have the lowest temperature. As the temperature falls along the range in which the polymer is highly elastic, the polymer’s resistance to stretching grows (stretching deformations decrease). This happens due to the strengthening of the intermolecular interactions due to lower thermal vibrations of the macromolecular segments. As a result, by setting up an uneven temperature distribution for the prepared material, it is possible to ensure the required thickness on any section of the product, having significantly increased the evenness of its thickness or durability of its sections most likely to be under physical stress.

However, the wide assortment of polymeric materials, multitude of configurations of forming tools caused by the multitude of product configurations, and missing information about the object all complicate the task of controlling product thickness distribution. The information incompleteness is mainly due to the large material surface temperature measurement error, as well as the inability to measure internal temperature of the material. In actual production, thermoforming modes for every type of product are chosen from experience. This leads to quite a lot of resource and energy consumption, and the selected temperature distributions don’t generally lead to products of required thickness distribution. During mass production, a technologist performs periodic inspections of thickness variation by measuring thickness distributions of no less than three items per batch. Such inspections only allow recording defects due to deviation from set thickness bounds, but don’t help prevent them. Defects during discrete unit production become an unrecoverable emergency situation. It’s necessary to provide production personnel with a flexible software tool for establishing cause-effect relationships in the control object and performing quality control of multi-assortment formed products. The development of software tool requires a complex approach based on knowledge of the peculiarities of thermoforming, product types, their quality indices and production modes, as well as application of mathematical modeling methods and information technologies.

Currently existing software solutions for modeling thermoforming (PAM-FORM, T-SIM, T-FORMCAD, POLYFLOW) allow calculating wall thickness distribution of the formed products and temperature distribution of the polymeric material during forming. The practice of using the software solutions for modeling various types of thermoforming techniques, designing appropriate equipment types and forming tools confirms their high efficiency and compliance with the level of modern production. However, the software solutions are only vaguely applicable to solving quality control tasks, as they do not allow calculating barrier characteristics of products, have complicated interfaces for production personnel, all at a relatively high cost. There are software solutions for designing configurations and calculating barrier characteristics of blister packs, whose mathematical core consists of models based on universal geometric modeling systems. An example of such an approach
is Pentapharm® BlisterPro®, created by Klöckner Pentaplast, an international corporation producing high-tech polymeric film [3]. Its mathematical core is a modeling system called Rhino. The key disadvantages of this approach are the need for extra training in 3D modeling and lack of a way to calculate limit values of water vapor and oxygen permeability through the blister as a result of calculating only the average thickness without taking into account thickness variation, which can be up to 30%.

There are mathematical models of thermoforming based on the law of conservation of mass that are described in relevant literature [4–6]. They enable calculating the wall thickness distribution along the height for various axisymmetric products of varied configurations and stretch ratios produced via pneumatic, vacuum or mechanical forming. The process of forming products is presented as a series of short-term even stretching of free sections, and bringing infinitesimally small sections of the heated material in contact with the relatively cold walls of the matrix. This contact leads to deformation suddenly halting as a result of the formation of a thin stiff outer layer on the surface of the material. However, due to the assumptions made about the uniform character of free section thinning, material profile shape during the forming stages, and heat uniformity in the material, these models cannot describe thermoforming adequately. Furthermore, the stretching and cooling coefficients for the polymer materials need to be experimentally established for every material type, each clamping frame–matrix radius ratio, and for different heat conditions for a process. Since these models are independent of material behavior, they give poor predictions of wall thickness distribution, even for simple product configurations like truncated cones. An alternative approach to solving the vacuum forming modeling task is presented in [7], where the main analysis tool is plasticity theory applied to finite deformations. The model is based on using one static equation of the theory of momentless thin membranes, and physical equations for the relationship between stresses and strains for a planar stressed state. Disadvantages of the proposed approach include disregarding strain rates’ influence on stresses, as well as having to use experimental values of the strain field for key components, and their use to calculate the stresses using physical equations. A more general approach to analyzing deformation processes during thermoforming is using mechanical models of polymeric materials [8–13]. These models describe the influence of deformation properties on stretching resistance. Examples of this approach include models based on momentless thin membrane approximation, describing plug assisted stretching using Ogden’s model [8, 9] and power law model [10]. However, the model proposed in [8] does not take into account the influence of the materials’ thermal state or the influence of the rate of stretching deformation on resistance to it. The model proposed in [10] does not contain criteria of or a procedure for verifying calculation results, consisting of the comparison between membrane volume and prepared material volume at each step of the stretching process. In [12, 13], we see a proposed model for the pneumatic forming of axisymmetric products that uses prior mechanical stretching of the prepared material. In order to describe the material’s behavior during stretching, a viscoelastic model is used. The model enables calculating wall thickness distribution of the formed products based on the geometric parameters of the forming tools, punch speed, and relaxation time. However, the model does not take into account stretch deformation in the circumferential direction.

Thus, there is no one modeling method that would allow us to offer a complex quality evaluation (thickness, barrier characteristics) for formed products depending on regime parameters of the process, various polymer types, and product configuration, that would account for not only forming the prepared materials, but their prior heating as well.

As a result, the goal of this article is to solve the pressing issue of developing a software solution that would use a library of mathematical models of thermal and deformation processes occurring during thermoforming to determine necessary regime parameters at key stages of the process that would ensure required product quality given various types of polymeric materials and products’ geometric parameters.

2. Formed product quality analysis and control problem statement. Software package structure

Analysis of the types of polymeric materials, heating and stretching methods, and product assortment
has enabled us to propose a description of thermoforming as a control object (figure 1). It presents itself as a series of vectors of input parameters \( X \), control actions \( U \), and output parameters \( Y \).

Figure 1. Informational description of thermoforming as a control object.

Most formed products used for packaging pharmaceutical or food products are axisymmetric bodies of various side profiles. The number of size types \( G_{prod} \) for packages is dominated by those shaped like cylinders or truncated cones (with top and bottom radii of \( R_{pr}^t \) and \( R_{pr}^b \)). This is confirmed with an analysis of the product lines produced using equipment made by ILLIG Maschinenbau (Germany), MEAF Machines B.V. (Netherlands), Tong Shin Pack (South Korea) companies et al.

The input parameters of the key stages of the process \( X_1 \) and \( X_2 \) are parameters of the prepared polymeric material \( X_{pm1} \) and \( X_{pm2} \), clamping frame parameters \( X_{fr} \), heater parameters \( X_{heat} \), and forming tool parameters \( X_{form} \). Polymeric materials produced via extrusion and calendering differ among each other in the thickness \( \delta_0 \) (film when \( \delta_0 \leq 0.5 \) mm, sheet when \( \delta_0 > 0.5 \) mm) and type of the polymer used \( T_{polym} \). Blisters for pills are made from polymeric film based on non-plasticized polyvinylchloride (PVC), polyethylene terephthalate (PET), and polypropylene (PP). Containers for food products are made from film and sheets based on polystyrene (PS), PVC, PET, and PP. The type of polymer determines thermal characteristics \( P_{therm} \) (density \( \rho \), specific heat \( c \), thermal conductivity \( \lambda \), and emissivity \( \varepsilon \)) and mechanical characteristics \( P_{mech} \) (resistance to stretching \( \mu_0 \) at reference temperature \( T_r \), influence degree of strain hardening on the resistance coefficient \( m \), influence degree of deformation rate intensity on the resistance coefficient \( n \), temperature coefficient \( b \)) of the polymeric material. The key thermoforming stages that determine production cycle time and resulting quality are heating the fixed polymeric material from a starting temperature \( T_0 \) to the temperature at which it is highly elastic (for amorphous polymers) or temperature at which the crystallites begin to melt (for crystalline polymers) due to thermal conductivity, as well as stretching of the heated material into the matrix and forming the product via biaxial stretching under normal stresses. The material is fastened in place with the clamping frame, which has an inner radius \( R_0 \), width \( \Delta_0 \), and temperature \( T_0 \). Heating the polymeric material is generally done in a radiative (with open infrared heaters) and convective
(with thermally sealed chambers hot air is fed into) way. For rigid (PVC, PP, PS) and thick sheet materials, radiation heating is recommended [2]. The top and bottom heater, enabling multi-zone heating necessary to achieve an uneven radial temperature profile of the material, have \( n_t \) heat zones each. Each heat zone has a radius \( R_{zl} \). The heaters’ emissivity is characterized with an emissivity coefficient \( \varepsilon_h \). The convective method, which produces more even heating of the material along its thickness, is characterized by a much longer time to reach a heated state (5–10 times that with the radiation method), which significantly lowers the process productivity. Furthermore, the convective method does not allow for multi-zone heating. The main method for forming rigid or thick-sheet materials is mechanical forming, which is applicable should the degree of stretching (ratio between product height \( H_m \) and its average nominal diameter) be greater than 0.5. It consists of stretching the fixed material with a punch of radius \( R_p \) into a matrix of radius \( R \) and height \( H \).

The heating and forming methods determine the possible control actions at the thermoforming stages. The heating stage control actions \( U_1 \) are heat zone temperatures of top and bottom heaters \( T_{zl}, T_{lb} \), and heating time \( \tau_h \). At the forming stage, the control actions \( U_2 \) are punch speed \( v_p \), which defines the forming speed.

After heating (\( t = \tau_h \)) the polymeric material, characterized by an uneven temperature field (having a temperature \( T_r \) distributed along its radius and thickness), is passed onto the forming stage. Here, over time \( \tau_s \) (\( 0 \leq \tau \leq \tau_s \)), the material is formed into product by stretching it in the meridional and circumferential direction (deformations \( \varepsilon_m, \varepsilon_c \), rates of deformations \( s_m, s_c \)) under corresponding normal stresses \( \sigma_m, \sigma_c \), occurring as a result of punch pushing. The resulting membrane has thickness \( \delta \), which changes along the radial coordinate \( r \) and over time \( t \). The product is characterized by quality indicators \( Q_{prod} \) – the radial thickness profile \( \delta_r \) and thickness variation index \( D_p \).

Based on the informational description of thermoforming, we form the problems of quality analysis and control of the formed products useable as packaging.

The quality analysis problem consists of using a mathematical model to analyze thermoforming so as to establish the influence of prepared material thickness \( \delta_b \), polymer type \( T_{polym} \), heater parameters \( X_{heat} \), forming tool parameters \( X_{form} \), control actions during heating \( U_1 \) and forming \( U_2 \) on the formed products’ quality indicators \( Q_{prod} \).

The quality control problem consists of the following: given certain input parameters \( X \) and using the thermoforming mathematical model, find such values for the control actions within their permissible ranges \( U \in [U^{\text{min}}; U^{\text{max}}] \) that would ensure the resulting product meets the presented quality requirements:

- thickness uniformity \( D_b \leq D_b^{\text{max}} \), guaranteeing uniform product permeability (without regions of lacking or excess water vapor and oxygen permeability), if the product is to be used for pharmaceutical packaging;
- preset radial thickness profile \( ||\delta' - \delta_{r0}|| \leq \Delta_b \), that would guarantee, for example, an increased durability of certain regions, if the product is meant for food packaging, where \( D_b^{\text{max}} \) is the maximum permitted thickness variation (%); \( \delta' = f(r) \) is the specified radial thickness profile (m); \( \Delta_b \) is the maximal permitted thickness profile deviation from the task (%).

In order to solve the presented problems, we’ve developed a software package. Its functional structure is presented in figure 2. The package includes a subsystem for modeling thermoforming, a databank of thermoforming characteristics, and an interface for the forming personnel and an administrator. Using their interface, the forming personnel inputs the prepared material characteristics \( \delta_b, T_{polym}, T_{lb} \), product geometric parameters \( G_{prod} \), clamping frame \( X_d \) and heater \( X_{heat} \) Parameters, and product use conditions \( C_{permeab} \) (required for calculating barrier properties). The vector \( C_{permeab} \) includes permeability analysis time \( \tau_p \), pressure drop between the two sides of the product wall \( \Delta p \), and external temperature \( T_{env} \). To configure the package for a specific polymer type \( T_{polym} \) and product geometric parameters \( G_{prod} \) we’ve developed the databank that includes updateable databases of polymer property parameters, forming tool geometric parameters and permissible ranges for control actions. The databases are relational. These databases are used to establish the values for polymers’ thermal properties.
and mechanical properties $P_{\text{therm}}$ and $P_{\text{mech}}$, the coefficients of polymer permeability to water vapor and oxygen $P_{\text{permeab}} = \{k_W, k_O\}$, the geometric parameters of the matrix and punch $X_{\text{form}}$ (per the following rule: $R = R_{pr}^1, H = H_{pr}, R_p = R_{pr}^b$), and control actions’ permissible value bounds $U_{\text{min}}, U_{\text{max}}$. The forming personnel performs a computational experiment, varying the control actions $U$ within the permitted range given preset input parameters $X$. In order to perform a new computational experiment, the forming personnel alters input parameters (polymer type, product geometric parameters, or number/radius of heating zones, for example).

The calculation of output parameters $Y_{\text{heat}}, Y$ is done using the thermoforming mathematical model, which is assembled using key stage models, which are based on the theory of thermal conductivity of solids, the laws of thermal radiation, the theory of momentless thin membranes and the laws of rheology as applied to polymers. To calculate barrier properties $Q_W, Q_O$ we use diffusion permeability models based on Fick’s first law for penetrant flow density.

To get complete information about the occurring thermal and deformational processes and analyze cause-effect relationships for the object, the forming personnel’s interface presents:
• tables and 3D graphs of temperature distribution along the radius and thickness of the polymeric material at various points in time during the heating stage, including at its end;
• tables and 3D graphs of stress, deformation, deformation rate, and membrane thickness distributions along the radial coordinate and over time during the forming stage;
• tables and 2D graphs of the formed product’s thickness profile along the radial coordinate and wall length coordinate (if the forming personnel mouses over a point on the 2D graph, the forming personnel will see the values of spatial coordinate (radial coordinate or wall length coordinate) and thickness at that point).

The calculated values for temperature, stresses, deformations, rates of deformations, and thickness are output into tables and onto graphs with spatial coordinate and time steps defined by the forming personnel.

Color visualizations of the calculated temperature and thickness distributions are created using the RGB color space, as it is the most appropriate to color detection by the human eye [14]. Color coordinates corresponding to calculated values of state parameter \(y – \) temperature \(T_i\) (thickness \(\delta_{yi}\)), are calculated using Lagrange interpolation polynomials:

\[ R_y = \sum_{i=0}^{I} R_{yi} \psi_i(\tilde{y}), \ G_y = \sum_{i=0}^{I} G_{yi} \psi_i(\tilde{y}), \ B_y = \sum_{i=0}^{I} B_{yi} \psi_i(\tilde{y}), \ \psi_i(\tilde{y}) = \prod_{j=0, j \neq i}^{I} \frac{\tilde{y} - \tilde{y}_j}{\tilde{y}_i - \tilde{y}_j} \]

where \(\tilde{y}\) is the normalized value of parameter \(y\); \(y_{\text{min}}, y_{\text{max}}\) are the minimal and maximal values of parameter \(y\); \(I\) is the number of regions which we break up the range of parameter \(\tilde{y}\) change into (usually, \(I = 7\)); \(R_{yi}, G_{yi}, B_{yi}\) are color coordinates, corresponding to the value \(\tilde{y}_i\) in the \(i\)-th interpolation node.

To visualize the temperature distribution, the relationship between color coordinates and boundary values of parameter \(\tilde{y}\) are set up with \(R_{y0} = G_{y0} = 0, B_{y0} = 255\) for \(\tilde{y}_0\) \((T_i = T_i^{\text{min}})\) and \(R_{yf} = 255, G_{yf} = B_{yf} = 0\) for \(\tilde{y}_f\) \((T_i = T_i^{\text{max}})\), so blue color corresponds to the least heated region of the prepared material, and red to the most heated. When visualizing the product thickness distribution \(R_{y0} = 255, G_{y0} = B_{y0} = 0\) for \(\tilde{y}_0\) \((\delta_{yi} = \delta_{yi}^{\text{min}})\) and \(R_{yf} = G_{yf} = 0, B_{yf} = 255\) for \(\tilde{y}_f\) \((\delta_{yi} = \delta_{yi}^{\text{max}})\), so red color corresponds to the thinnest regions of the product and blue to the thickest.

Transforming state parameter values into color coordinates enables us to visualize temperature and thickness distributions as colored 3D models of prepared material and product, presented in the forming personnel’s interface and configurable with geometric parameters \(\delta_{hi}, R_{hi}, G_{pol}.\)

The software package enables creating a report regarding the performed computational experiment and exports the input data \(\{G_{\text{prod}}, X, U^{\text{min}}, U^{\text{max}}, U, C_{\text{permeab}}\}\) and calculation results (array of output values \(\{Y_{\text{mean}}, Y, Q_{w}, Q_{o}\}\)) into Excel.

The software package is developing using the following computer tools: IDE Visual Studio (using C#); database management system SQLite; CAD system 3ds Max (for building 3D models of prepared materials and products).

3. Mathematical models for heating and forming polymeric materials, and product permeability

The library of mathematical models for key stages of thermoforming includes models describing double-sided radiation (single-zone and multi-zone) heating of polymeric materials and biaxial stretching of heated materials during mechanical forming. The models require configuring for the specific polymer type and resulting product’s geometric parameters.

During development of the heating and forming models, the following assumptions were made, their presence strongly substantiated by literature on modeling polymeric material thermoforming:

• the prepared material is a round cylinder with a radius of \(R_0\) and height of \(\delta_{hi}\) which is used during the forming stage to create an axisymmetric hollow product, which takes the shape of a cylinder or truncated cone;
• the main mechanism of heat transfer from the heated surfaces of the prepared material into the
polymer mass is thermal conductivity;

- the polymer’s thermal characteristics are independent of its temperature \( T \) (so, the change in polymer density within the 20–200 °C range is insignificant and constitutes 3–15 %);
- the heat zone temperatures are kept constant by a stabilizing system;
- the temperature of the prepared material’s edge located between the top and bottom part of the clamping frame \( (R_0 < r \leq R_0 + \Delta_0) \) is the same as the temperature of the frame, which is kept constant during the heating stage;
- the heat transfer from the prepared materials’ surface to the air in the space between the heaters and the prepared material is negligibly small;
- the prepared material is firmly locked in place by the clamping frame, and material locked in place by the clamping frame does not stretch into the matrix (the rate of deformation in the circumferential direction at a clamped point is zero);
- the temperature of the prepared material does not change (isothermal process) due to the briefness of the forming stage (forming time, and resultingly time spent in contact with the punch, generally constitutes 1–3 s), low thermal conductivity \((0.12–0.29 \text{ W m}^{-1} \text{ °C}^{-1})\) of thermoplastic, and the use of a thermally insulating coating on the punch that increases its thermal resistance on the contact surface;
- the polymer is incompressible, as Poisson ratio is near 0.5 for polymers in highly elastic state; the polymer’s anisotropic characteristics due to orientational stretching of its macromolecules are minor;
- the curvature of the material membrane during forming is negligible; this is justified by the degree of curvature falls as the punch radius grows, and as a rule for this task the radius ratio of punch to matrix is 0.5–0.8;
- due to the thinness and flexibility of the membrane, it is in a momentless planar stress state (no bend, normal stresses in the meridional and circumferential directions that are uniformly distributed across the thickness of the membrane in each cross-section, normal stress in the perpendicular direction to the membrane surface and shear stresses are negligibly small);
- the inertial and mass forces are minor due to the loss mass of the membrane and small (10–200 mm/s) average forming speeds;
- the mechanical model of the polymer is assembled by generalizing (based on Ilyushin’s postulate on the proportionality of deviators of stress tensor and deformation rate tensor for isotropic materials) results of experiments on monaxial stretching performed in various deformation-temperature modes to the case of a planar stress state that takes into account the near monotone character of deformation development \([6, 8, 10, 15]\).

The heating model includes a thermal conductivity equation, initial condition and boundary conditions, which describe heat transfer between the prepared material and the clamping frame, between the prepared material and the multi-zone heaters (while taking into account the repeated reflection of heat rays off the surface of the prepared material):

\[
p_{\text{c}} \frac{\partial T}{\partial t} = \lambda \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) + \frac{\partial^2 T}{\partial z^2} \right], \quad 0 < r < R_0, \quad 0 < z < \delta_0, \quad 0 < t \leq \tau_h \tag{1}
\]

\[
T\big|_{t=0} = T_0, \quad 0 \leq r \leq R_0, \quad 0 \leq z \leq \delta_0
\]

\[
\left. \frac{\partial T}{\partial r} \right|_{r=0} = 0, \quad \left. -\left( \lambda \frac{\partial T}{\partial r} \right) \right|_{r=R_0} = \frac{T\big|_{r=R_0} - T_h}{\xi}, \quad \xi = \frac{A_h}{\lambda}, \quad 0 \leq z \leq \delta_0, \quad 0 < t \leq \tau_h \tag{3}
\]

\[
-\left( \lambda \frac{\partial T}{\partial z} \right)\big|_{z=0} = \sigma_0 F_k \left( (T_{zh} + 273)^4 - (T|_{z=0} + 273)^4 \right), \quad F_k = \frac{\varepsilon \varepsilon_h}{\varepsilon - \varepsilon \varepsilon_h + \varepsilon_h} \tag{4}
\]
\[- \left( \frac{\partial T}{\partial z} \right)_{0 \rightarrow -\infty} = \sigma_c F_c \left[ (T_{1 \rightarrow 0} + 273) - (T_{1 \rightarrow -\infty} + 273)^4 \right] \tag{5} \]

where \( t \) is time (s); \( r \) is the coordinate along the prepared materials’ radius (m); \( z \) is the coordinate along the thickness of the prepared material (m); \( \xi \) is the thermal resistance of the prepared material edge located in the clamping frame (\( \text{m}^2 \cdot \text{C} \cdot \text{W}^{-1} \)); \( \sigma_0 \) is the Stefan–Boltzmann constant (\( \text{W} \cdot \text{m}^{-2} \cdot \text{K}^{-4} \)); \( F_\varepsilon \) is the emissivity coefficient.

Model (1)–(5) enables us to calculate the temperature distribution along the radius and thickness of the prepared material at every moment during the heating stage \( T(r, z, t) \), and determine the temperature distribution at the end of the heating stage \( T_f = T(r, z, \tau) \) resulting from the control actions \( U_i \) for a given set of input parameters \( X_i \). An implicit finite-difference variable directions method (Peaceman–Rachford scheme) was used for this calculation, which provides unconditional stability, second-order precision and cost-effective computing [16]. It consists of splitting the finite-difference equation approximating equation (1) into two half-steps which in sum proved a full step in time. The linearization of the finite-difference analogues of boundary conditions (4), (5) occurs by breaking down the non-linear temperature functions into a Taylor series while conserving the linear terms and approximating the temperature derivatives as right differences (forward differences). The systems of linear algebra equations we get at each half-step in time have tridiagonal coefficient matrices with diagonal dominance, and as a result in order to solve them we use the highly effective Thomas algorithm. In order to check the results for convergence, we cut the grid steps in half and compare temperature distributions calculated on progressively finer grids. The temperature distribution at the end of the heating process is used to calculate the stretching resistance coefficient for the polymeric material.

The forming model includes equations for calculating membrane thickness and polymeric material stretch deformation, equations for the balance of stretch forces and deformation continuity, a mechanical model for the polymer and a geometric model for the membrane, as well as boundary conditions:

\[ \delta = \delta_0 \exp \left[ - \left( \epsilon_m + \epsilon_c \right) \right], \quad 0 \leq r_i \leq R, \quad 0 \leq t \leq \tau \]

\[ \frac{ds_m}{dt} = s_m, \quad 0 \leq r_i \leq R, \quad 0 < t \leq \tau, \quad \epsilon_c = \ln \left( \frac{r_i}{r} \right), \quad 0 < r_i \leq R, \quad 0 \leq t \leq \tau \tag{7} \]

\[ \frac{d(\sigma_m - \sigma_m)}{dr_i} = \frac{\sigma_c (\sigma_m - \sigma_m)}{r_i}, \quad 0 < r_i < R, \quad 0 < t \leq \tau \tag{8} \]

\[ r_i \frac{ds_c}{dr_i} = s_m - s_c - 0.5 \nu_p \sin (2\alpha_c) \frac{R - R_p}{R - R_p}, \quad 0 < r_i < R, \quad 0 < t \leq \tau \tag{9} \]

\[ \sigma_m - \sigma_c = 2 \bar{\mu} I_c^{n-1} s_m, \quad \sigma_c - \sigma_c = 2 \bar{\mu} I_c^{n-1} s_c, \quad \sigma = \left( \sigma_m + \sigma_c \right)/3 \tag{10} \]

\[ \bar{\mu} = \left( \int_0^s \mu \, dz \right)^{1/3}, \quad \mu = \mu_0 I_c^{n} \exp \left[ -b(T_r - T_i) \right], \quad 0 \leq r_i \leq R, \quad 0 \leq t \leq \tau \tag{11} \]

\[ I_c = 2 \sqrt{s^2_m + s_m s_c + s^2_c}, \quad I_c = 2 \sqrt{s^2_m + \epsilon_m s_c + \epsilon^2_c} \tag{12} \]

\[ \frac{dr}{dr} = \exp (\epsilon_m) \sin \alpha_c, \quad 0 < r \leq R, \quad 0 \leq t \leq \tau \tag{13} \]
\[ \alpha_i = \arctg \left[ \frac{R - R_p}{v \sqrt{f + \left( R - R_p \right) \left( \tan \theta \right)^{-1}}} \right], \quad R_p < r_i \leq R \]  

\[ V_t = 2\pi \left[ \int_0^{R_t} r \delta dr + \int_{R_t}^R \left( r + 0.5\delta \right) \delta \left( \sin \alpha \right)^{-1} dr \right], \quad 0 \leq t \leq \tau_s \]  

\[ \delta \left( \sin \alpha \right)^{-1} \bigg|_{r_0} = \delta \bigg|_{r_1}, \quad 0 \leq r_0 < R \leq r_1 \]  

\[ \delta \left( \sin \alpha \right)^{-1} \bigg|_{r_1} = \delta \bigg|_{r_2}, \quad 0 \leq r_1 < R \leq r_2 \]  

\[ \delta \left( \sin \alpha \right)^{-1} \bigg|_{R} = \delta \bigg|_{R}, \quad 0 \leq r \leq R \]  

where \( r_i \) is the radial coordinate of the current location of the membrane’s material points (in the Lagrange coordinate system) (m); \( \alpha_i \) is the current angle between the side walls of the membrane and the matrix (for the part of the membrane making contact with the punch \( \alpha_i = \pi/2 \); when \( t = 0 \), \( \alpha_i = \alpha_{0_i} \), that is, an assumption is made that the initial material stretching is uniform) (rad); \( \overline{\sigma} \) is the average stress (Pa); \( \overline{\mu} \) is the stretch resistance coefficient, averaged over the membrane’s thickness (Pa·s\(^6\)); \( I_s \) is the quadratic invariant of the deformation rate tensor (s\(^{-1}\)); \( I_{m} \) is the quadratic invariant of the deformation tensor (the degree of polymeric material deformation hardening when stretched); \( V_t \) is the current membrane volume (m\(^3\)); \( \delta_{\text{m0}} \) is the meridional deformation of the material at the beginning; \( \sigma_{\text{m0}} \) is the stress at the point of anchorage in the clamping frame (Pa).

The initial condition (16) is attained because at the initial point in time, corresponding to a minor turning angle \( \alpha_0 \) for the part of the membrane not in contact with the punch, the material’s deformation corresponds to a minor uniform reduction in membrane thickness

\[ \delta \left( \sin \alpha \right)^{-1} \bigg|_{r_0} = \delta \bigg|_{r_1}, \quad 0 \leq r_0 < R \leq r_1 \]  

\[ \delta \left( \sin \alpha \right)^{-1} \bigg|_{r_1} = \delta \bigg|_{r_2}, \quad 0 \leq r_1 < R \leq r_2 \]  

\[ \delta \left( \sin \alpha \right)^{-1} \bigg|_{R} = \delta \bigg|_{R}, \quad 0 \leq r \leq R \]  

The boundary condition (17) when \( r_1 = 0 \) is attained from the experimentally verified assumption about the uniformity of deformation near the center of the contacting region of the membrane. This is accomplished by coating the punch with a low-friction material.

Model (6)–(17) enables us to calculate the distributions of stress-deformation state characteristics and thickness \( \delta(r, t) \) of the membrane along the radial coordinate at every point in time during the forming stage, and determine the distribution of product thickness \( \delta_{\text{m0}} = \delta(r, \tau_s) \) in relation to the control actions \( U_2 \) per a given set of input parameters \( X_2 \) and \( Y_{\text{heat}} \). This is difficult to calculate due to the nonlinearity of the equations for the polymer’s mechanical model (10)–(12) and lack of information about stress \( \sigma_{\text{m0}} \) at the boundary condition (17) when \( r_1 = R \). As a result, we use an iterative method to solve the model’s equations. The search for stress \( \sigma_{\text{m0}} \) at each step in time concludes once the deformation uniformity condition (the boundary condition (17) when \( r_1 = 0 \)) is met. During the stress \( \sigma_{\text{m0}} \) search loop, we calculate the radial distribution of deformations, thickness, deformation rates, and stresses of the membrane at that point in time. We use Euler’s method to convert the differential equations (8), (9), (13) into algebra equations. We use the same step size we used to calculate the temperature distribution \( T_t \) as our initial step size along the radial coordinate. The deformation rate in the meridional direction \( \delta_m \) is calculated by solving the mechanical model equations together via Newton’s method, which guarantees quadratic speed of iteration convergence. The results’ validity is verified by satisfying the polymeric material incompressibility condition, characterized by the value of difference between current volume of the membrane \( V_n \), calculated via formula (15), and the prepared material volume [17]. If the incompressibility condition is not met, then steps along the radial coordinate and time are halved and calculation is repeated.

We use the product’s thickness distribution \( \delta_{\text{m0}} \) to calculate the thickness variation index \( D_\text{m0} \), water vapor permeability \( Q_\text{w} \), and oxygen permeability \( Q_0 \).
\[
D_\delta = \left(1 - \frac{\delta_{\min}^m}{\delta_{\min}^p}\right) 100, \quad Q_W = k_W F_{pr} \delta_{pr}^{-1} \Delta p r_p, \quad Q_O = k_O F_{pr} \delta_{pr}^{-1} \Delta p r_p
\] (18)

where \( \delta_{\min}^m, \delta_{\min}^p \) is the minimal and average thickness (m); \( k_W, k_O \) is the coefficient of water vapor permeability (kg m\(^{-1}\) Pa\(^{-1}\) s\(^{-1}\)) and oxygen permeability (m\(^2\) Pa\(^{-1}\) s\(^{-1}\)) of the polymer, which characterize the process speed and depend first and foremost on external temperature \( T_{env} \); \( F_{pr} \) is the product surface area (m\(^2\)).

Formulas for calculating barrier characteristics (18) are attained by integrating Fick’s first law equations along the thickness of the product for the flow densities of corresponding penetrants (water vapor, oxygen). The hollow thin-walled product is approximated by a plate of equal diffusion resistance with the same geometric parameters (thickness, surface area) as the product. Assumptions about the stationary nature of the penetrant stream are permitted (which can be achieved with a constant pressure drop across the thickness of the product). Furthermore, an assumption about the dependence of penetrant equilibrium concentration in solid solution on partial pressure as per an analogue of Henry’s law is also permitted [3].

4. Results and discussion

The thermoforming mathematical model was verified by comparing the measured and calculated thickness distributions for truncated cone shaped packages. The packages are characterized by their geometric parameters (blister for pills, packaging for milk products), and are made from various polymer types (PVC, PS) using single-zone or multi-zone heating at various temperatures for the heaters’ heating zones, and various forming speeds. The mean squared deviation of the calculated thickness distributions from the measured thickness distributions was 1–3 %, which falls within permitted measurement error for thickness measurement and shows the model is adequate.

In figure 3 we show the results of temperature and thickness calculations given two-zone heating \((R_{h1} = 20 \text{ mm, } T_{h1} = T_{b1} = 310 \ ^\circ\text{C, } R_{h2} = 80 \text{ mm, } T_{h2} = T_{b2} = 325 \ ^\circ\text{C})\) and mechanical forming \((R_{pr}^A = 50 \text{ mm, } H_{pr} = 50 \text{ mm, } R_{pr}^B = 20 \text{ mm, } v_p = 10 \text{ mm s}^{-1})\) of a PS sheet \((\delta_0 = 1 \text{ mm, } T_0 = 20 \ ^\circ\text{C})\).

![Figure 3](image-url)

**Figure 3.** Distributions of polymeric material state parameters at thermoforming stages.

Lowering the heating in the first heating zone, which heated the most deformable region of the polymeric material during forming (the region that makes contact with the punch) led to a loss of temperature of this material region, which results in an increase in the stretching resistance coefficient in that zone, which leads to a lower deformation intensity and the corresponding increase in membrane thickness. This leads to a drop in the unevenness of the product thickness distribution \((D_\delta = 21 \ %; \text{ figure 4})\) which helps ensure a more uniform product permeability \((Q_W = 82 \text{ mg, } Q_O = 1371 \text{ mm}^3 \text{ for } \tau_p = 24 \text{ h, } \Delta p = 0.1 \text{ MPa, } T_{env} = 23 \ ^\circ\text{C})\).

Analyzing the modeling results allows us to select a rational thermoforming regime which ensures
quality requirements for products of given type are met.

**Figure 4.** Product wall thickness distribution for truncated cone shaped product.

5. Conclusion

We’ve developed a library of mathematical models for the process of production and use of hollow volume products used as packaging materials, which includes models describing two-sided radiation heating and biaxial stretching of polymeric materials during mechanical forming and models describing permeability of various types of penetrants through formed product walls. The mathematical models can be configured for a specific type of polymer as well as geometric parameters and use conditions of the product, and can be used to calculate quality indicators (thickness distribution, thickness variation index, barrier properties) resulting from specific control actions at key stages of thermoforming.

We’ve developed a configurable software package which enables us to use mathematical models to solve the problem of analyzing the influence of polymeric material characteristics and forming tool parameters on the resulting products’ quality indicators. It also allows us to find a rational thermoforming regime which can guarantee required quality indicators are met in a multi-assortment production.

Including this software package in the production control system when producing multi-assortment hollow volume products made of polymeric materials via thermoforming enables an increase in production effectiveness due to product quality increase, defect decrease, as well as conservation of resources and energy. The software package can be used (provided the applicable database and mathematical model library extension) to aid in controlling the forming process in analogous high-tech productions (for example, production of sound-dampening products from polymer-textile materials for cars).

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